

## MO 11: Posters 2: Novelties in Molecular Physics: Femtosecond Spectroscopy, Quantum Control, Electronic Spectroscopy, Biomolecules and Photochemistry

Time: Tuesday 16:30–19:00

Location: Empore Lichthof

MO 11.1 Tue 16:30 Empore Lichthof

**Relaxation and dissociation dynamics of XUV induced wavepackets in polyatomic molecules** — ●GEERT REITSMA, MARTIN GALBRAITH, LORENZ DRESCHER, JOHAN HUMMERT, MARC VRAKING, OLEG KORNILOV, and JOCHEN MIKOSCH — Max-Born-Institut, Berlin, Germany

The combination of ultrafast science with advanced spectroscopic techniques, like mass spectrometry, velocity map imaging, and transient absorption spectroscopy, offers an excellent opportunity to gain knowledge on relaxation and dissociation dynamics in polyatomic molecules. However, in ultrafast science, one always has to reach a compromise between the optimal spectral and the optimal temporal resolution. At the same time this also triggers an intriguing question: To which extent does the coherence of the excitation process influence the molecular response? To address this question, we employ two HHG beamlines: one attosecond beamline providing <5fs time resolution with an intrinsically broad spectrum, and one monochromator beamline providing a 300 meV spectral resolution with a 30fs time-resolution. The attosecond beamline was used to measure photodissociation timescales of methyl iodine and iodobenzene by means of transient absorption spectroscopy, mainly making use of the broad spectrum of the ultrashort XUV-pulses. We measured non-adiabatic relaxation timescales of electron-correlation states in benzene and polycyclic aromatic hydrocarbons by means of time-resolved mass spectrometry. The monochromator beamline will be employed to obtain complementary data for selected harmonics.

MO 11.2 Tue 16:30 Empore Lichthof

**Investigation of the transient absorption of the adsorbate in contact with different metallic surfaces** — ●ALIREZA MAZAHERI TEHRANI, FAEZEH MOHAGHEGH, and ARNULF MATERNY — Physics and Earth Sciences, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The interactions of molecules adsorbed on metal surfaces with surface plasmon polaritons are of great importance for spectroscopic applications, such as surface enhanced Raman spectroscopy (SERS). So far, experimental SERS investigations have mostly been performed in the frequency domain using continuous wave lasers. This way, although the results are quite interesting concerning applications, they mostly fail to nicely address the underlying physical concepts and mechanisms of SERS. Time-resolved experiments, however, would help us to gain a better understanding of the underlying energy transfer mechanisms involved in surface enhanced spectroscopy due to different time scale characteristics of the adsorbate in various configurations. In this work we investigate the transient absorption of the adsorbate in contact with different metallic surfaces. Surface plasmons polaritons are excited with a femtosecond laser pulse (Pump) adjusted to the ground state absorption. Dynamic information of the system can then be probed by another time-delayed femtosecond laser pulse, which can freely be adjusted to other excited states of adsorbates or to the ground state absorption. This experiment provides us with a much deeper insight into the energy transfer mechanisms between SPPs and molecules.

MO 11.3 Tue 16:30 Empore Lichthof

**Direct Observation of Excited State Chirality in Formic Acid** — YAN YANG<sup>1</sup>, HARAMRIT K. GILL<sup>1</sup>, ●MARTIN PITZER<sup>1,2</sup>, MAXSIM KUNITSKI<sup>1</sup>, TILL JAHNKE<sup>1</sup>, REINHARD DÖRNER<sup>1</sup>, and MARKUS SCHÖFFLER<sup>1</sup> — <sup>1</sup>Institut für Kernphysik, Goethe-Universität Frankfurt am Main — <sup>2</sup>Experimentalphysik IV, Universität Kassel

In this contribution, we present first results on a laser-induced excitation of the planar molecule formic acid (HCOOH) into a chiral excited state. As the energy barrier between the left-handed and right-handed forms (enantiomers) is generally lower in excited states than for chiral molecules in the ground state, the tunneling between the two enantiomers is expected to occur on timescales observable in a pump-probe setup. Measuring the tunneling time can help to detect a possible effect of parity violation in chiral molecules [1]. Formic acid molecules are among the most simple examples with a chiral  $\pi^*$  state [2]. Excitation into this state is accomplished by a femtosecond laser pulse and the handedness is probed by Coulomb Explosion Imaging, using a COLTRIMS-setup (Cold Target Recoil Ion Momentum Spectroscopy)

[3,4]. Different excitation energies and pump-probe schemes are employed in order to investigate the temporal behaviour of the excited molecule.

- [1] R. Berger, Phys. Chem. Chem. Phys. 5 (2003), 12-17
- [2] T.L. Ng and S. Bell, J. Mol. Spec. 50 (1974), 166-181
- [3] M. Pitzer, et al., Science 341 (2013), 1096-1100
- [4] R. Dörner, et al., Phys. Rep., 330 (2000), 95-192

MO 11.4 Tue 16:30 Empore Lichthof

**Collinear two-dimensional spectroscopy via fluorescence detection with shot-to-shot phase cycling** — ●SIMON DRAEGER<sup>1</sup>, SEBASTIAN ROEDING<sup>1</sup>, JAKUB DOSTÁL<sup>1</sup>, ANDREAS STEINBACHER<sup>1</sup>, PATRICK NUERNBERGER<sup>2</sup>, and TOBIAS BRIKNER<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — <sup>2</sup>Physikalische Chemie II, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum

Coherent multidimensional spectroscopy is a powerful tool to study electronic couplings and coherences of molecular systems. We present a novel all-collinear setup to perform pulse-shaper-assisted two-dimensional electronic spectroscopy with fluorescence detection. The variation of the interpulse delays and their relative phases (phase cycling) is performed shot-to-shot with a pulse shaper (Dazzler, Fastlite) with 1 kHz rate, enabling a rapid data acquisition. We show data of a 4-pulse excitation of cresyl violet in the liquid phase and compare it with data acquired in the non-collinear BOXCAR geometry. With the applied acquisition scheme, rephasing and non-rephasing contributions can be extracted from one single measurement session via phase cycling.

MO 11.5 Tue 16:30 Empore Lichthof

**Photoinduced processes of bilins in solution and as protein-bound cofactor** — ●DANIEL MUSCHOL<sup>1</sup>, MAXIMILIAN THEISS<sup>1</sup>, PATRICK SINGER<sup>1</sup>, NICOLE FRANKENBERG-DINKEL<sup>2</sup>, TILMAN LAMPARTER<sup>3</sup>, and ROLF DILLER<sup>1</sup> — <sup>1</sup>Dept. of Physics — <sup>2</sup>Dept. of Biology, Univ. Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>3</sup>Botanical Inst., Karlsruhe Inst. of Techn., 76131 Karlsruhe, Germany

Bilins are linear tetrapyrroles with rich and diverse photochemistry in solution, involving C-C single- and double-bond isomerization of one or several of the pyrrole-pyrrole methine bridges. When bound as cofactor to plant phytochrome proteins they serve as chromophores for a photoinduced signal cascade enabling red-light sensing and a variety of essential biological processes, such as seed germination, shade avoidance and photomorphogenesis. In the bound form protein-chromophore interaction restricts the potentially possible degrees of freedom and guides the excited electronic state dynamics along a complex reaction coordinate involving both chromophore as well as protein contributions, including H-bond networks and protein bound water molecules. For a better understanding of these mechanisms for molecular reaction control we study the primary photochemistry of the bilins biliverdin (BV), phycocyanobilin (PCB) and bilirubin (BR) in solution and of the BV-binding bathy-phytochromes Agp2 (*Agrobacterium fabrum*) and PaBphP (*Pseudomonas aeruginosa*) employing fs transient absorption in the UV/Vis and mid-IR spectral region. In particular, Agp2 shows strongly pH dependent primary reaction kinetics suggesting excited state proton transfer processes.

MO 11.6 Tue 16:30 Empore Lichthof

**Robust control of molecular excitation using GDD-TOD-shaped femtosecond laser pulses** — ●HENDRIKE BRAUN<sup>1</sup>, TIM BAYER<sup>2</sup>, CRISTIAN SARPE<sup>1</sup>, MATTHIAS WOLLENHAUPT<sup>2</sup>, and THOMAS BAUMERT<sup>1</sup> — <sup>1</sup>Universität Kassel, Institut für Physik und CINSaT, 34132 Kassel, Germany — <sup>2</sup>Carl von Ossietzky Universität Oldenburg, Institut für Physik, 26129 Oldenburg, Germany

We report on adiabatic population control in molecules using intense shaped femtosecond laser pulses. The laser pulses employed are spectrally phase-shaped using a combination of second and third order dispersion [1]. The resulting pulses offer a variety of different temporal amplitude and phase shapes to optimally adapt to the laser-induced intramolecular excitation dynamics [2,3]. Third order dispersion (TOD) results in temporally asymmetric pulses featuring gentle slopes as well

as rapidly varying amplitude profiles. Group delay dispersion (GDD) provides time-dependent frequency sweeps being essential for adiabatic control scenarios [4]. In our experiments we investigate the interaction of GDD-TOD-shaped pulses with potassium molecules serving as a prototype system for coherent control scenarios. We support our experimental studies by quantum dynamics simulations in order to model the interaction processes and extract the quantum control mechanisms at play.

- [1] J. Schneider *et al.*, Phys. Chem. Chem. Phys. **13**, 8733 (2011)  
 [2] H. Braun *et al.*, J. Phys. B **47**, 124015 (2014)  
 [3] T. Bayer *et al.*, Adv. Chem. Physics, accepted  
 [4] N. Vitanov *et al.*, Annu. Rev. Phys. Chem. **52**, 763 (2001)

MO 11.7 Tue 16:30 Empore Lichthof

**Optimisation of strong laser field-free alignment using tailored light fields** — ●EVANGELOS THOMAS KARAMATSKOS<sup>1,2</sup>, TERRY MULLINS<sup>1</sup>, SEBASTIAN TRIPPEL<sup>1</sup>, ROSARIO GONZÁLEZ-FÉREZ<sup>3</sup>, ARNAUD ROUZÉE<sup>4</sup>, and JOCHEN KÜPPER<sup>1,2,5</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY — <sup>2</sup>Department of Physics, University of Hamburg — <sup>3</sup>Instituto Carlos I, Universidad de Granada — <sup>4</sup>Max Born Institute, Berlin — <sup>5</sup>The Hamburg Center for Ultrafast Imaging, University of Hamburg

Laser induced electron diffraction and molecular frame photoelectron angular distribution measurements have emerged as potential new techniques for imaging molecular structure and dynamics. Control over the rotational motion of molecules represents the first step towards this goal. Here, we present a combined theoretical and experimental effort to optimise the degree of laser field-free alignment of molecules in the gas phase. We start by solving the time-dependent Schrödinger equation for a rigid rotor in interaction with a non-resonant laser field and a static electric field [2] and use an iterative learning-loop algorithm to determine the ideal pulse shape that optimises the degree of alignment. These calculations serve as a guide to complement the experiments where the temporal profile of the alignment laser pulse is optimally tailored using a spatial light modulator in a feedback loop, using the same evolutionary strategies as in the simulations. We discuss the simulation results and the experimental realization on the example of the linear molecule OCS. [1] Stapelfeldt *et al.*, Rev. Mod. Phys. **75**, 543 (2003) [2] Omiste *et al.*, J. Chem. Phys. **135**, 064310 (2011)

MO 11.8 Tue 16:30 Empore Lichthof

**Cavity-controlled ultracold chemistry** — ●TOBIAS KAMPSCHULTE<sup>1</sup>, ANDREAS KÖHN<sup>2</sup>, and JOHANNES HECKER DENSCHLAG<sup>1</sup> — <sup>1</sup>Inst. f. Quantenmaterie, Universität Ulm — <sup>2</sup>Inst. f. Theoretische Chemie, Universität Stuttgart

Ultracold molecules can be formed from ultracold atoms by photoassociation involving a spontaneous emission process, resulting in a number of final states. Here we want to use strong coupling to an optical cavity to selectively enhance the creation of a certain final state. During this process, a photon will be emitted into the cavity mode which can be detected. A collective enhancement of the effect would enable “superradiant chemistry”. Furthermore, we propose using the cavity as a non-destructive detector for ultracold molecules, i.e. by avoiding photon scattering. Finally, we present realistic parameters for cavities and how to integrate them into an existing cold-atom setup.

MO 11.9 Tue 16:30 Empore Lichthof

**Strong-field ionization of HD molecules with two-color laser pulses** — ●YONGHAO MI, NICOLAS CAMUS, MARTIN LAUX, LUTZ FECHNER, ROBERT MOSHAMMER, and THOMAS PFEIFER — Max-Planck-Institute for Nuclear Physics

Single and double ionization of HD molecules as well as fragmentation and Coulomb-explosion in strong two-color laser pulses (800 nm + 400 nm) have been studied utilizing a reaction-microscope. Asymmetries in the emission directions of both electrons and ions are analyzed as a function of the relative phase between the two fields and differences between the various fragmentation-channels are discussed in terms of possible ionization pathways.

MO 11.10 Tue 16:30 Empore Lichthof

**Non-adiabatic dynamics and Dynamic Stark Effect: Wave-packet confinement and induced photon emission in alkali halides.** — ●SIMONA SCHEIT<sup>1</sup>, YASUKI ARASAKI<sup>2</sup>, YUTA MIZUNO<sup>2</sup>, and KAZUO TAKATSUKA<sup>2</sup> — <sup>1</sup>Theoretische Chemie, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg — <sup>2</sup>Department of Basic Science, Graduate School of Arts and Sciences, University of

Tokyo, Komaba, 153-8902, Tokyo, Japan

The two lowest Sigma states of alkali halides with their characteristic avoided crossing can be diabaticized in such a way that the two resulting diabatic states are those of minimum and maximum intrinsic dipole moment. Taking as example the LiF molecule it will be shown that, by shining a strong continuous non-resonant driving field in the visible, the non-adiabatic dynamics can be controlled by exploiting the Dynamic Stark Effect in such a way that the nuclear wave packet is trapped in the region of the crossing. The result is a back and forth transition between diabatic states of very different intrinsic dipole moments, with consequent fast oscillations in the molecular dipole moment resulting in the emission of dipole radiation with characteristic high harmonics structure. The effect of molecular rotation on the photoemission spectrum will be investigated, as well as the mechanism of wave-packet confinement, which leads to a complete suppression of photodissociation.

MO 11.11 Tue 16:30 Empore Lichthof

**Angle-resolved spectroscopy of electron emissions by chiral molecules** — ●JAN DREISMANN and STEFAN SCHIPPERS — AG Atom- und Molekülphysik, Justus-Liebig-Universität Gießen

Chirality of molecules is of essential importance to their effect in chemical reactions. The understanding of the importance of chiral molecules in biology and medicine is growing. However the physical properties of chiral systems are not well-known until now. There are many open questions like the chirality’s influence on the molecules’ atomic structure and electron dynamics. Interactions of polarized photons or electrons with chiral molecules can give insights in this unknown physics.

An electron spectrometer ESA-22 with angular resolution is used for analysis of electrons from these reactions. Electrons emitted in the spectrometers scattering plane pass electrostatic electrodes for energy separation and then are detected on 22 channel-electron-multipliers. Changes to the existing setup had to be made for using an molecular gas target and an electron beam instead of a photon beam.

We present first experimental spectra of Methyl lactate ( $C_4H_8O_3$ ) taken after the refurbishments. Electron impact on this molecule leads to fragmentation thus we observe angle resolved Auger spectra for the main components oxygen and carbon.

MO 11.12 Tue 16:30 Empore Lichthof

**Study of the self-reaction products of propargyl radicals via IR/UV ion-dip-spectroscopy** — ●FLORIAN HIRSCH<sup>1</sup>, PHILIPP CONSTANTINIDIS<sup>1</sup>, INGO FISCHER<sup>1</sup>, and ARGHYA DEY<sup>2</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Department of Molecular and Laser Physics, Institute for Molecules and Materials, Radboud University Nijmegen, 6525 AJ Nijmegen, Netherlands

The self-reaction products of propargyl radicals produced by flash pyrolysis have been studied by ion-dip-spectroscopy in a free jet. On the basis of the high stability of these radicals, it has been assumed for years that they might play an important role in the formation of polycyclic aromatic hydrocarbons (PAHs) and consequently soot.

The spectroscopic method utilized in this study is capable of providing mass selective infrared spectra, which can be used for unambiguous identification of the formed molecules. The radicals have been generated by flash pyrolysis from the bromide precursor and ionized at fixed wavelengths between 263 - 275 nm. A tunable free electron laser provided infrared radiation in the range of 550 - 1750 cm<sup>-1</sup>. Subsequent analysis of the differences in ion signals, with and without infrared excitation, resulted in the sought after infrared spectra. Eventually comparison with theoretical and experimental data was performed for identification of the various reaction products.

This poster will provide a fundamental overview of methodology and results of this study, executed at the Free Electron Laser for Infrared eXperiments (FELIX) (Nijmegen, Netherlands).

MO 11.13 Tue 16:30 Empore Lichthof

**Why Did Nobody Report on Single-Molecule Experiments on FMO Yet?** — ●ALEXANDER LÖHNER<sup>1</sup>, KHURAM ASHRAF<sup>2</sup>, RICHARD COGDELL<sup>2</sup>, and JÜRGEN KÖHLER<sup>1</sup> — <sup>1</sup>Experimental Physics IV and Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Germany — <sup>2</sup>Institute of Molecular, Cell & Systems Biology, College of Medical Veterinary and Life Sciences, University of Glasgow, United Kingdom

In green-sulfur bacteria sunlight is absorbed by chlorosomes and transferred to the RC via the Fenna-Matthews-Olson (FMO) complex.

FMO consists of three monomers each accommodating eight BChl a molecules, and was the first pigment-protein complex for which the structure has been determined with atomic resolution [1]. Since then this complex has been the subject of numerous studies both experimentally and theoretically.

Here we report about fluorescence-excitation spectroscopy as well as emission spectroscopy from individual FMO complexes at low temperatures. It appears that the FMO complexes are subjected to very fast spectral fluctuations resulting in spectra that resemble those from ensembles that were recorded under the same experimental conditions. In other words, on the time scales that are experimentally accessible by single-molecule techniques the FMO complex features an ergodic behaviour.

[1] Fenna, Matthews, Nature 258 (1975), 573

MO 11.14 Tue 16:30 Empore Lichthof

**Investigation of synergetic effects on the photophysics of functional molecules in solvent mixtures** — ●CHRISTIAN SPIES, CLAUDIO BEAKOVIĆ, BASTIAN GEISSLER, and PATRICK NUERNBERGER — Ruhr-University Bochum, Physical Chemistry II, Bochum, Germany

Several molecules are well known for their solvent-dependent photochromism, for instance spiropyrans can usually be switched by UV-light to a merocyanine form which absorbs in the visible spectral region. [1,2] The absorption wavelength, as well as the thermal ground-state relaxation rate into the spiro-form, shows synergetic effects in some solvent mixtures. [3,4] A synergetic effect causes a property of the solute to be higher or lower compared to each of the neat solvents. In this contribution we employ a systematic approach to analyze this kind of behavior in more detail to disclose which solvent and solute parameters are important for a synergetic effect to emerge. Steady-state as well as ultrafast time-resolved measurements in different solvent mixtures shed light on the interactions and dynamics in solution. It turns out that the occurrence of synergetic effects depends on a complex interplay between solvent-solvent and solvent-solute interactions. [1] J.B. Flannery, J. Am. Chem. Soc. 90 (1968), 5660. [2] C. Lenoble et al., J. Phys. Chem. 90 (1986), 62. [3] P. Jacques, Chem. Phys. Lett. 171 (1990), 353. [4] M. Rosés et al., J. Chem. Soc., Perkin Trans. 8 (1995), 1607.

MO 11.15 Tue 16:30 Empore Lichthof

**Time-resolved fluorescence of 2-dimensional crystals of LH2 complexes** — ●INGA ELVERS<sup>1</sup>, PU QIAN<sup>2</sup>, NEIL HUNTER<sup>2</sup>, RICHARD HILDNER<sup>1</sup>, and JÜRGEN KÖHLER<sup>1</sup> — <sup>1</sup>Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — <sup>2</sup>Department of Molecular Biology and Biotechnology, University of Sheffield, Sheffield S10 2TN, United Kingdom

We investigate the fluorescence kinetics and energy transport properties of artificially arranged arrays of light-harvesting2 (LH2) complexes. The LH2 complexes were extracted from the purple bacterium *Rba. sphaeroides* and crystallised into 2-dimensional sheet-like or tubular crystals using a lipid from *E. Coli*. Employing a versatile streak-camera setup, we investigate the fluorescence kinetics of these arrays as a function of the excitation fluence and the repetition rate. We find that the lifetime of both samples are significantly shorter with respect to samples consisting of isolated LH2 complexes. Furthermore, the fluorescence decays of the arrays strongly depend on the variation of the excitation fluence and the repetition rate. These observations indicate the occurrence of exciton-exciton annihilation processes and allows to study the energy transfer dynamics within these arrays.

MO 11.16 Tue 16:30 Empore Lichthof

**Design of an Experimental Setup for Optical Gating with Single Molecules** — ●JOHANNES MAIER<sup>1</sup>, TINA WELLER<sup>2</sup>, MUKUNDAN THELAKKAT<sup>2</sup>, MARTTI PÄRS<sup>1</sup>, and JÜRGEN KÖHLER<sup>1</sup> — <sup>1</sup>Experimental Physics IV and Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Germany — <sup>2</sup>Applied Functional Polymers, University of Bayreuth, Germany

Photochromic molecules can be interconverted between two metastable states by light [1-3]. We synthesized a triad consisting of a photochromic unit (Dithienylperfluorocyclopentene, DCP) and two highly fluorescent chromophores (Perylene Bisimide, PBI) and monitored the PBI fluorescence intensity as a function of the state of the DCP. To ensure sufficiently long observation times for the study of individual triads we had to achieve both an enhanced photostability and an improvement of the light collection optics. The former was accomplished by performing the experiments at cryogenic temperatures, and for the latter we resorted to solid immersion lens (SIL) optics [4], which yielded

an enhancement of the light collection efficiency by a factor of 1.8 with respect to the situation without the SIL. In first experiments we demonstrate distinctive changes of the fluorescence intensity emitted from individual triads triggered by changing the state of the DCP.

[1] Hirshberg: C. R. Hebd. Seances Acad. Sci. 1950, 231, 903 [2] Pärs, Hofmann, Willinger, Bauer, Thelakkat, Köhler: Angew. Chem. Int. Ed. 50 (2011), 11405 [3] Pärs, Gräf, Bauer, Thelakkat, Köhler: APL 103(2013), 221115 [4] Jasny, Sepiol, Irgartinger, Traber, Renn, Wild: Rev. Sci. Instrum. 67(1996), 1425

MO 11.17 Tue 16:30 Empore Lichthof

**A molecular movie of Interatomic Coulombic Decay in NeKr** — ●FLORIAN TRINTER<sup>1</sup>, TSVETA MITEVA<sup>2</sup>, MIRIAM WELLER<sup>1</sup>, SEBASTIAN ALBRECHT<sup>1</sup>, ALEXANDER HARTUNG<sup>1</sup>, MARTIN RICHTER<sup>1</sup>, JOSHUA WILLIAMS<sup>1</sup>, AVERELL GATTON<sup>3</sup>, BISHWANATH GAIRE<sup>3</sup>, THORSTEN WEBER<sup>3</sup>, JAMES SARTOR<sup>4</sup>, ALLEN LANDERS<sup>4</sup>, BEN BERRY<sup>5</sup>, VASIL STUMPF<sup>2</sup>, KIRILL GOKHBERG<sup>2</sup>, REINHARD DÖRNER<sup>1</sup>, and TILL JAHNKE<sup>1</sup> — <sup>1</sup>Institut für Kernphysik, Goethe-Universität, 60348 Frankfurt am Main, Germany — <sup>2</sup>Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, 69120 Heidelberg, Germany — <sup>3</sup>Lawrence Berkeley National Laboratory, Chemical Sciences Division, Berkeley, California 94720, USA — <sup>4</sup>Department of Physics, Auburn University, Auburn, Alabama 36849, USA — <sup>5</sup>J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA

During the last 15 years a novel decay mechanism of excited atoms has been discovered and investigated. This so called "Interatomic Coulombic Decay" (ICD) involves the chemical environment of the electronically excited atom or molecule: the excitation energy is transferred to a neighbor of the initially excited particle usually ionizing that neighbor. It turned out that ICD is a very common decay route in nature as it occurs across van der Waals and hydrogen bonds. The time evolution of ICD is predicted to be highly complex, as its efficiency strongly depends on the distance of the atoms involved and this distance typically changes during the decay. Here we present a direct measurement of the temporal evolution of ICD using a novel experimental approach.

MO 11.18 Tue 16:30 Empore Lichthof

**Time-Resolved Step-Scan FTIR and Transient Absorption/Reflection Investigations on a Dinuclear Cu(I)-NHETPHOS-complex** — ●MANUEL ZIMMER<sup>1</sup>, FABIAN DIETRICH<sup>1</sup>, FLORIAN BÄPPLER<sup>1</sup>, MANUELA WALLECH<sup>2</sup>, DANIEL VOLZ<sup>3</sup>, STEFAN BRÄSE<sup>2</sup>, ROLF DILLER<sup>1</sup>, and MARKUS GERHARDS<sup>1</sup> — <sup>1</sup>TU Kaiserslautern, 67663 Kaiserslautern — <sup>2</sup>Karlsruhe Institute of Technology, 76131 Karlsruhe — <sup>3</sup>cynora GmbH, 76646 Bruchsal

Time-resolved (TR) infrared experiments enable the investigation of chemical reactions, photochemical/-physical processes and their kinetic traces. With the step-scan technique we are able to identify electronically excited states and excited state structures by comparison with theoretical results from quantum chemical calculations. Here we present the first TR step-scan FTIR measurements on a dimetallic Cu(I)-NHETPHOS-complex in a KBr matrix. These complexes which are developed for emitter material in OLEDs are a very promising substitute for currently used Ir-complexes. We show the capabilities of step-scan FTIR measurements as well as femtosecond transient absorption and reflection measurements in a KBr matrix and thin films. Time-resolved IR spectra of electronically excited states have been obtained and in combination with quantum chemical calculations we could characterize the molecular structure of the electronic T<sub>1</sub>-state (with a lifetime of about 2 μs). Wavelength and temperature dependent measurements have been performed to gain detailed information about the excited state processes and deactivation mechanisms.

MO 11.19 Tue 16:30 Empore Lichthof

**A setup for time- and frequency resolved kinetic terahertz absorption spectroscopy using temperature jumps** — ●CLAUDIUS HOBERG — Ruhr-Universität Bochum

The constant rearrangement of hydrogen bonds in the water network occurs on picosecond timescales having their spectral signatures in the THz frequencies. Solvents like salts and biomolecules are known to alter these picosecond motions of the hydrogen bond network. By using temperature jumps we induce non-equilibrium conditions in samples and monitor the kinetic response of the hydrogen bond network. The time-domain THz setup utilizes direct digitization of signals, rapid scanning techniques together with a temperature controlled sample cell. The setup provides a time resolution of 0.5 μs in the spectral range between 0.3 and 2.5 THz and a dynamic range of about 70 dB.