

MO 7: Poster 1

Time: Thursday 17:30–19:30

Location: P

MO 7.1 Thu 17:30 P

Multiple-quantum coherence signals in thermal vapors — ●FRIEDEMANN LANDMESSER, ULRICH BANGERT, LUKAS BRUDER, MARCEL BINZ, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

We investigate collective effects in thermal atomic alkali vapors by multiple-quantum coherence experiments, where multiphoton processes can be separated from one-photon transitions and can be assigned to specific particle numbers [1,2]. We extended our previous collinear phase-modulated electronic coherent spectroscopy scheme [1] from a 2-pulse to a 4-pulse sequence [2]. The technique is sensitive enough to reveal weak interparticle interactions, despite the thermal motion and the spatial separation of the atoms in the micrometer-range [3]. First results of fluorescence measurements of a potassium vapor will be presented.

[1] L. Bruder et al., Phys. Rev. A 92, 053412 (2015).

[2] S. Yu et al., Opt. Lett. 44, 2795 (2019).

[3] L. Bruder et al., Phys. Chem. Chem. Phys. 21, 2276 (2019).

MO 7.2 Thu 17:30 P

Compression of deep ultraviolet femtosecond pulses using self-phase modulation in bulk material — ●PHILLIP WOSCHNIK, LUKAS BRUDER, ULRICH BANGERT, and FRANK STIENKEMEIER — Institute of Physics University of Freiburg

In many laboratories deep ultraviolet (DUV) pulses at 266 nm are generated by third-harmonic generation of a Ti:Sa femtosecond laser output. Compressing these pulses to short durations is difficult, especially if the pulse duration of the Ti:Sa laser is in the range of > 100 fs. Riedle and co-workers have demonstrated a facile scheme based on self-phase modulation in bulk material, which permits compression of the DUV pulses to < 50 fs [1]. We adapt this scheme in our laboratory and will present the concept and first results.

[1] N. Krebs, I. Pugliesi, and E. Riedle, Pulse Compression of Ultrashort UV Pulses by Self-Phase Modulation in Bulk Material, Appl. Sci. 3, 153 (2013).

MO 7.3 Thu 17:30 P

Dynamics of photo-excited cesium atoms attached to helium nanodroplets — ●N. RENDLER¹, A. SCOGNAMIGLIO¹, M. BARRANCO^{2,3}, M. PF^{2,3}, N. HALBERSTADT⁴, K. DULITZ¹, and F. STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg — ²Departament FQA, Faculty of Physics, University of Barcelona — ³Institute of Nanoscience and Nanotechnology, University of Barcelona — ⁴Laboratoire des Collisions, Agrégats, Réactivité, Paul Sabatier University

Due to the exceptional capability to isolate atoms, molecules and complexes and owing to the inertness of superfluid He, He nanodroplet isolation spectroscopy is a powerful technique to investigate molecular structure and dynamics. However, the low-perturbative character of the He environment is challenged for electronically excited or ionized dopant species. Various processes can be triggered by the electronic excitation and ionization of the dopant. For example, the ejection of electronically excited atoms can take place along with electronic relaxation induced by the He environment [1]. Additionally, He-dopant exciplexes can form due to the pairwise He-dopant interaction [2]. We present an experimental study of the time-resolved dynamics of photo-excited Cs atoms attached to He droplets [3]. The timescales for desorption and re-adsorption as well as for CsHe exciplex formation are determined for the 6p states of Cs using femtosecond pump-probe velocity-map-imaging spectroscopy and ion-time-of-flight spectrometry [3]. Our results are compared to time-dependant density-functional theory simulations published earlier [4].

[1] Loginov et al., J. Phys. Chem. A 111, 7504-7515, (2007)

[2] Reho et al., Faraday Discuss, 108, 161-174, (1997)

[3] Rendler et al., arXiv:2106.12330

[4] Coppens et al., Eur. Phys. J. D 73, 94, (2019)

MO 7.4 Thu 17:30 P

Probing of a vibrational wave packet in the electronic ground state of methyl p-tolyl sulfoxide via time-resolved photoelectron circular dichroism — ●NICOLAS LADDA¹, MAX WATERS², VÍT SVOBODA², MIKHAIL BELOZERTSOV², SUDHEENDRAN VASUDEVAN¹,

SIMON RANECKY¹, TONIO ROSEN¹, SAGNIK DAS¹, JAYANTA GHOSH¹, HANGYEOL LEE¹, HENDRIKE BRAUN¹, THOMAS BAUMERT¹, HANS JAKOB WÖRNER², and ARNE SENFTLEBEN¹ — ¹Institut für Physik, Universität Kassel, 34132 Kassel, Germany — ²Laboratorium für Physikalische Chemie, ETH Zürich, 8093Zürich, Switzerland

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

MO 7.5 Thu 17:30 P

Chirp and intensity dependence of the circular dichroism in ion yield of 3-methylcyclopentanone measured with femtosecond laser pulses — ●SAGNIK DAS, JAYANTA GHOSH, TOM RING, 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[1,2]. We use our home-built Time of Flight (ToF) mass spectrometer with our recently established twin peak[3] measurement setup to study the effect of linear chirp (GDD) on the anisotropy. The candidate molecule for this experiment is 3-methylcyclopentanone (3-MCP). In the study we present here, we perform all the experiments at 309 nm, where 3-MCP shows high 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 observe enhancement of anisotropy for chirped pulses, which we compare to band-width limited pulses of equal peak intensity.

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

[2] H. G. Breunig et al., ChemPhysChem, 10, 1199, 2009

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

MO 7.6 Thu 17:30 P

Exciton Dynamics in Squaraine-based Thin Films — ●STEFFEN WOLTER¹, MANUELA SCHIEK², and STEFAN LOCHBRUNNER¹ — ¹Institute of Physics, University of Rostock, 18051 Rostock, Germany — ²Institute of Physics, Carl von Ossietzky University of Oldenburg, 26111 Oldenburg, Germany

Squaraine dyes are promising candidates for light harvesting electron donor materials in small molecule solar cells, since they combine strong absorption in the visible spectral region with a high stability compared to other organic compounds like low bandgap polymers. Bulk-heterojunction solar cells based on squaraine:fullerene blends have been shown to suffer from low mobility and recombination losses [1]. In depth understanding of the loss mechanism requires investigation of fundamental processes upon light absorption on ultra-fast time scales. In this contribution, the light induced processes in different squaraine based thin films are investigated by femtosecond pump-probe spectroscopy. The dynamics in pure films of 2,4-bis[4-(N,Ndiisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQIB) is studied to obtain a picture of the possible electronic relaxation pathways in the donor material. In a next step, the results are compared to films of SQIB blended with a fullerene acceptor (PCBM). Strong differences in the kinetics and the spectral signatures are observed and attributed to the population of charge separated states.

[1] Scheunemann, Kolloge, Wilken, Mack, Parisi, Schulz, Lützen, Schiek. Appl. Phys. Lett. 111 (2017) 183502.

MO 7.7 Thu 17:30 P

Photoelectron circular dichroism of heavier chalcogenofenones using near-ultraviolet femtosecond laser pulses — ●SUDHEENDRAN VASUDEVAN¹, MANJINDER KOUR², SIMON.T. RANECKY¹, SAGNIK DAS¹, JAYANTA GHOSH¹, DENIS KARGIN¹, NICOLAS LADDA¹, HANGYEOL LEE¹, TONIO ROSEN¹, IGOR VINDANOVIC¹, THOMAS BAUMERT¹, ROBERT BERGER², HENDRIKE BRAUN¹, THOMAS.F. GIESEN¹, RUDOLF PIETSCHNIG¹, and ARNE SENFTLEBEN¹ — ¹Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Philipps Universität Marburg, Hans-Meerwein Str.4, 35032 Marburg, Germany

Photoelectron spectra and photoelectron circular dichroism (PECD) measurements after femtosecond laser resonance enhanced multiphoton ionization (2+1 REMPI) are reported for chalcogenofenones with variation of the chalcogen atom from oxygen to sulfur and selenium. Short pulses allow for excitation and ionization of the intermediate states out of an almost frozen nuclear configuration and reduce the influence of internal conversion processes. Keeping the excitation wavelength fixed, the contributing resonances and ionization energies are tuned in a bathochromic fashion by chemical substitution of heavier atoms. Intermediate electronic states excited during the REMPI process are assigned based on the measured photoelectron spectra and ab initio quantum chemical calculations. The bathochromic shifts cause the heavier chalcogenofenones to have absorption in the visible region, which opens the door for future laser excitation, and control studies on the important fenchone prototype.

MO 7.8 Thu 17:30 P

Two-dimensional electronic spectroscopy of phthalocyanine on rare gas clusters — ●ULRICH BANGERT, LUKAS BRUDER, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Two-dimensional electronic spectroscopy (2DES) is an ideal tool to study dynamics with a high spectral-temporal resolution. With recent advances of 2DES towards the gas phase, versatile samples like rare gas cluster beams have become accessible [1]. Rare gas clusters doped with multiple molecules act as miniature cryostats hosting well defined many body systems. Previous experiments on the spectroscopy and life-time measurements of such systems have provided valuable details about singlet fission and superradiance in acene molecules [2,3].

We apply 2DES to this approach and study free-base phthalocyanine in two different environments: embedded in superfluid helium nanodroplets and deposited on the surface of solid neon clusters. First results show 2D spectra of organic molecules with unprecedented spectral resolution and reveal details of the cluster environment, including the homogenous linewidth of 0.42 cm^{-1} on neon clusters.

[1] L. Bruder et al., J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).

[2] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).

[3] M. Müller et al., Phys. Rev. B 92 (12), 121408 (2015).

MO 7.9 Thu 17:30 P

Probing electronic dynamics in the pentacene-C₆₀ complex doped in helium nanodroplets — ●AUDREY SCOGNAMIGLIO, NICOLAS RENDLER, LUKAS BRUDER, KATRIN DULITZ, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder Straße 3a, 79104 Freiburg-im-Breisgau

The motivation to study the pentacene-C₆₀ complex arises from its relevance for organic photovoltaics (OPVs) research. OPVs are known to have high charge mobility¹ and are predicted to have higher quantum efficiencies than inorganic photovoltaics, by overcoming the Shockley-Queisser limit^{2,3}. The helium nanodroplet matrix isolation technique offers the unique possibility to synthesize complexes of organic molecules in their low-energy states, while the interaction with the droplet is negligible. Experimental and theoretical studies show that after excitation via the $S_0 \rightarrow S_1$ transition in pentacene, the charge is expected to transfer towards the exciton states of the complex within 100 fs to 5 ps^{4,5}. Our approach is to measure the charge transfer dynamics occurring within the Pc-C₆₀ complex embedded in helium nanodroplets by means of time-resolved two-color pump-probe spectroscopy using photoelectron imaging and ion time-of-flight spectroscopy.

[1] *Polym. Rev.* 52, 1(2012) [2] *Appl. Phys. Lett.* 95, 033301(2009) [3] *J. Am. Chem. Soc.* 132, 12698 (2010) [4] *Science* 334, 1541 (2011) [5] *J. Am. Chem. Soc.* 136, 1599 (2014)

MO 7.10 Thu 17:30 P

Intrinsic Electronic Dynamics of of Ru^{II}-Polypyridyl Complexes Studied by Ion Spectroscopy — ●ROUMANY ISRAÏL¹, LARS SCHÜSSLER³, PATRICK HÜTCHEN², WERNER THIEL², ROLF DILLER³, and CHRISTOPH RIEHN¹ — ¹FB Chemie, TU Kaiserslautern, Erwin-Schrödingerstr. 52 — ²FB Chemie, 54 — ³FB Physik, 46

Ru^{II}-polypyridyl complexes are featured in a wide range of applications in the areas of medicine (photoactivatable prodrugs) and material science (photovoltaics/catalysis). Tailored ligand design enables the control of their efficiency and photoactivity by tuning the relative energies of the ³MLCT and ³MC states. A selected series of Ru^{II}-polypyridyl complexes in the type of [Ru(y-bpy)₂(x-py)₂]²⁺ (bpy = (2,2-bi)pyridine), where x/y are varying substituents of different electronic donating/withdrawing character, were examined by a combination of mass spectrometry and laser spectroscopy in the frequency and time domain in an ion trap. Here, static absorption spectra were recorded by determining fragment ion yields as a function of laser wavelength (UV photodissociation spectra) and compared to TD-DFT calculations to characterize the electronic transitions. The femtosecond dynamics were elucidated via a pump-probe scheme recording excited-state lifetimes. Electron withdrawing substituents on the pyridine chromophore were found to destabilize the Ru^{II}-pyridine bond in the ground-state while stabilizing electronically excited-state ³MC. Electron-donating substituents on bpy are observed to stabilize the coordinative bond, while stabilizing the ³MLCT-state resulting in longer excited-state lifetimes.

MO 7.11 Thu 17:30 P

Photodissociation spectroscopy of binuclear coinage metal complexes — ●MARCEL SCHMITT¹, SEBASTIAN KRUPPA¹, SIMON WALG¹, WERNER THIEL¹, WIM KLOPPER², and CHRISTOPH RIEHN¹ — ¹Fachbereich Chemie und Forschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern — ²Institut für Physikalische Chemie, KIT, 76131 Karlsruhe

Multimetallic coinage metal complexes, featuring intricate metal-philic (M-M) interaction that govern photophysical properties such as bright luminescence and redox reactivity, are a prominent topic in functional material research [1,2]. Here, using quadrupole ion trap mass spectrometry, *in situ* synthesized homo- and heterobinuclear d¹⁰-d¹⁰ metal complexes of type [MM'(dcpm)₂]²⁺ (M, M' = Cu^I, Ag^I, Au^I; dcpm = bis(dicyclohexylphosphino)methane) were investigated in gas-phase via collisional-induced dissociation (CID) and ultraviolet photodissociation (UV PD) spectroscopy using femto- and nanosecond laser sources [3]. The resulting photodissociation spectra show a spectral blue shift of the lower energy metal-centered (MC) states in the order of Cu₂ < CuAu < CuAg < Au₂ < AgAu < Ag₂. These spectra were supported by quantum chemical calculations of *GW*-Bethe-Salpeter-equation (*GW*-BSE) approach, revealing a shortening of metal-metal binding upon excitation assigned to ¹MC(dσ*-pσ / dσ*-pπ) transitions.

[1] Q. Wan *et al.*, PNAS USA, 2021, 118 (1) e2019265118; [2] C.-M. Che *et al.*, Coord. Chem. Rev. 2005, 249, 1296; [3] S. V. Kruppa *et al.*, Phys. Chem. Chem. Phys. 2017, 19, 22785.

MO 7.12 Thu 17:30 P

Photofragmentation behaviour of small cationic silicon-oxide clusters — ●JULIAN VOSS, TAARNA STUEDEMUND, MARKO FÖRSTEL, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Deutschland

Interstellar dust plays a major role in the formation processes of stars and solar systems. The formation mechanisms of this dust are, however, still poorly understood. One molecular species found in interstellar matter is SiO [1] and we try to understand how and if such small Si and O containing molecules can play a role in the formation of large μm-sized silicate particles, a major component of interstellar dust [2]. In this study we focus on silicon-oxide species with two oxygen atoms per molecule. The investigated cations are generated by a laser vaporization source and their mass spectra are examined [3]. We furthermore gain insight into the molecular structure and the electronic properties of Si_nO₂⁺ by measuring their photon energy dependent photodissociation behaviour which is compared to quantum chemical TD-DFT calculations.

[1] R. Wilson *et al.*, 1971, *Astrophys. J.*, 167, L97

[2] B. A. Sargent *et al.*, 2009, *ApJ.*, 690, 1193

[3] M. Förstel *et al.*, 2017, *Rev. Sci. Instrum.*, 88, 123110

MO 7.13 Thu 17:30 P

Determination of the Enantiomeric Excess of Chiral Substances in Mixtures via Photoelectron Circular Dichroism — ●SIMON RANECKY¹, GIANNIS GIANNAKIDIS³, PETROS SAMARTZIS³, SUDHEENDRAN VASUDEVAN¹, HAN-GYEOL LEE¹, NICOLAS LADDA¹, TONIO ROSEN¹, SAGNIK DAS¹, JAYANTA GHOSH¹, HENDRIKE BRAUN¹, BARRATT PARK², TIM SCHÄFER², and THOMAS BAUMERT¹ — ¹Uni Kassel — ²Uni Göttingen — ³IESL-FORTH Iraklio (Greek)

The ionization of randomly oriented chiral molecules with circularly polarized light leads to an asymmetric angular photoelectron distribution. Depending on the handedness of the molecules and the sense of rotation of the incident light, more electrons are scattered forward or backward with respect to the direction of the incident light. This effect is called photoelectron circular dichroism (PECD). Its size can reach more than 10% for pure enantiomers and decreases for lower enantiomeric excesses (EE). It can be applied to determine the EE of chiral substances with a precision below 1% [1].

Tunable high resolution nanosecond lasers in combination with a cold molecular beam are a highly selective mean for ionization [2]. Here, we mixed fenchone and camphor with different EE and selectively ionized either fenchone or camphor by tuning the wavelength to the band origin of their B-band (2+1 REMPI-scheme with ca. 400 nm) and measured their background suppressed PECD. We report the results and an analysis of the EE of both substances in the mixture

[1] A. Kastner et al., ChemPhysChem, 17, 1119 - 1122, (2016)

[2] A. Kastner et al., Phys. Chem. Chem. Phys., 22, 7404, (2020)

MO 7.14 Thu 17:30 P

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

Quantum interference spectroscopy schemes are well established in the visible range to control and resolve the static properties and dynamics of quantum systems. Recently these principles got extended into the XUV regime [1,2]. Here acousto-optical modulators are used to achieve interferometric measurements supported by a phase cycling scheme. However, in this scheme a significant amount of material is introduced in the optical beam path at the fundamental frequency which prohibits using ultrashort pulses and high laser intensities. We present a new approach to achieve phase cycling while minimizing the amount of material dispersion by an order of magnitude. We will present the basic concept of this approach. The setup is commissioned and will be combined with a tabletop HHG source to conduct studies in the XUV regime.

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

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

MO 7.15 Thu 17:30 P

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

Quantum interference techniques such as wave packet interferometry (WPI) in the extreme ultraviolet (XUV) regime set the basis for advanced nonlinear spectroscopy methods, such as multidimensional spectroscopy. These methods are however very difficult to implement at short wavelengths due to the required high phase stability and sensitivity. Recently, we have overcome these difficulties and have introduced a concept to implement such experiments with XUV free-electron lasers [1]. We are now developing a new setup optimized for seeding tabletop high-harmonic generation sources. The setup is based on acousto-optic modulation of intense near infrared pulses. We will present the concept of the setup along with first characterization results.

1.*A. Wituschek et al., Tracking attosecond electronic coherences using phase-manipulated extreme ultraviolet pulses, Nature Communications, 11:883 (2020).

MO 7.16 Thu 17:30 P

Magnetic properties and their correlation to the electronic ground states of isolated trinuclear 3d spin frustrated complexes — ●MICHAEL LEMBACH¹, JOHANNES LANG¹, MAXIMILIAN LUCZAK¹, YANNICK MEES¹, ROUMANY ISRAÏL¹, VICENTE ZAMUDIO-BAYER², MARTIN TIMM², CHRISTINE BÜLOW², BERND VON ISSENDORFF⁴, AKIRA TERASAKI³, CHRISTOPH RIEHN¹, TOBIAS LAU², and GEREON NIEDNER-SCHATTEBURG¹ — ¹Technische Universität Kaiserslautern, Kaiserslautern, Germany — ²Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — ³Kyushu University, Fukuoka, Japan — ⁴Physikalisches Institut, Freiburg, Germany

Transition metal complexes often reveal extraordinary magnetic properties. In this case an assembly of spins located on an assembly of atoms cannot arrange their orientation in a way they can profit from the magnetic interaction with the neighbored spin. The electronics of $[\text{Fe}_3\text{O}(\text{CH}_3\text{CO}_2)_6\text{L}_{0-3}]^+$ (L = pyridine) complexes are extremely sensitive to intrinsic geometric distortions of the M_3O core induced by the bridging ligands and/or the axial ligands. We probe the magnetic moments and electronic transitions of these trinuclear complexes via X-Ray Magnetic Circular Dichroism (XMCD) and Ultra Violet Photon dissociation (UVPD) spectra as isolated molecule, to rule out packing effects or bulk ordering. Combining these techniques reveals that the coordination of axial pyridine ligands to the complex disturbs the triangular geometry of the Fe_3O core with a change in the ground state electronic structure and the magnetic exchange coupling.

MO 7.17 Thu 17:30 P

Photoelectron diffraction off conformer selected biomolecules — ●LUDMILA SCHNEIDER¹, MELBY JOHNY², HUBERTUS BROMBERGER², FLORIAN TRINTER³, SEBASTIAN TRIPPEL² und JOCHEN KÜPPER^{1,2,3} — ¹Department of Physics, Universität Hamburg — ²Center for Free-Electron Laser Science, Deutsches Elektronen Synchrotron DESY — ³Department of Physics, Goethe Universität Frankfurt

Angular measurements of photoelectrons gave us a whole new understanding of the inner structures of molecules. By investigating the recoil frame photoelectron angular distribution from molecules with a known orientation or by studying ion and electron appearance in coincidence, it is possible to reveal the geometry of the molecule. In our present work, we look at the molecule 3-chloro-phenol (3CP) an aromatic alcohol with a chlorine, with the use of a Reaction Microscope at PETRA III synchrotron light source. We obtained 3D velocity vectors of the chlorine atom of 3CP (using 250 to 500 eV light), in coincidence to the arrival of various ion fragments of 3CP. Ultimately, this will provide us with knowledge about the electronic and geometric structures of the cis and trans isomers of 3CP.

MO 7.18 Thu 17:30 P

Excitation transport in molecular aggregates with thermal motion — ●RITESH PANT and SEBASTIAN WÜSTER — Department of Physics, Indian Institute of Science Education and Research, Bhopal, Madhya Pradesh 462 066, India

One of the promising features of molecular aggregates is the transport of exciton energy over the long distance due to the Coulomb coupling. In our work we explore to what extent thermal motion of entire monomers can guide or enhance the excitation transport. We show that transport through motion can yield higher transport efficiencies in the presence of on-site energy disorder than the static counterpart for two simple models of molecular motion: (i) longitudinal vibrations along the aggregation direction (ii) torsional motion of planar monomers in a plane orthogonal to the aggregation direction. For both models we find parameter regimes in which the motion enhances excitation transport, however these are more realistic for the torsional scenario, due to the limited motional range in a typical Morse type inter-molecular potential. We finally show that the transport enhancement can be linked to adiabatic quantum dynamics. This transport enhancement through adiabatic motion appears a useful resource to combat exciton trapping by disorder. In the next step of this exploration, we include the effect of intramolecular vibrations and extend the quantum dynamics calculation for excitation transport to an open-quantum-system technique, a non-Markovian quantum state diffusion, which is an efficient method to study the effect of non-Markovian environment on excitation transport.

MO 7.19 Thu 17:30 P

Focused beams of small (bio-)nanoparticles from aerodynamic lens injectors — ●LENA WORBS^{1,2}, JANNIK LÜBKE^{1,2,3}, AMIT K. SAMANTA¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-

Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg

Determining structure and observing dynamics from isolated proteins and nanoparticles using x-ray diffractive single-particle imaging (SPI) requires sample-delivery and injection methods that provide one single particle per x-ray pulse in the interaction region. Aerodynamic-lens-stack (ALS) injectors have been used to deliver collimated and focused particle-beams for such experiments on larger nanoparticles (~50-100 nm) [1]. We extended the use and detection of particle beams toward smaller nanoparticles and present simulations and experiments on the performance of ALS injectors for 25 nm polystyrene spheres. This highlights the use of ALS injectors for small bio-nanoparticles. In addition, we present techniques to separate particles [2] according to charge caused by the aerosolization method employed. This paves the way toward pure beams of identical particles for SPI experiments.

[1] K. Ayyer, et al.; *Optica* **8**(1), 15-23 (2021)

[2] Y.-P. Chang, et al.; *Int. Rev. Phys. Chem.* **34**, 557-590 (2015)

MO 7.20 Thu 17:30 P

Charge migration in aminophenol following sub-fs X-Ray pulses: Influence of nuclear effects and the XFEL shot-to-shot variation — ●GILBERT GRELL^{1,2}, ZHAOHENG GUO³, AGOSTINO MARINELLI³, JAMES P. CRYAN³, ALICIA PALACIOS², and FERNANDO MARTÍN^{1,2} — ¹IMDEA Nanociencia, Madrid, 28049, Spain — ²Departamento de Química, Universidad Autónoma de Madrid, 28049, Spain — ³SLAC National Accelerator Laboratory, Menlo Park, 94025, CA, USA

Recently, it has been demonstrated at the LCLS facility that XFELs are capable of producing sub-fs soft X-Ray pulses. This makes it now possible to use tunable soft X-Ray pulses, with much higher intensity than their high harmonic generation counterparts, enabling non-linear spectroscopies to investigate attosecond electron dynamics in molecules. We here present theoretical results describing the ultrafast charge dynamics induced in the p-aminophenol molecule ionized with a sub-fs 260 eV pulse, i.e. below the carbon K-edge. The ionization calculations have been carried out using the static exchange B-spline DFT method that has been successfully applied in related studies at lower photon energies. In particular we scrutinize the influence of the shot-to-shot variation in terms of envelope, phase, and intensity by considering a set of 100 different X-Ray pulses obtained from start-to-end simulations of the XFEL. Moreover, we examine the ground state nuclear effects in the resulting charge fluctuations. To this end we take into account an ensemble of molecular geometries sampled from the equilibrium Wigner distribution.

MO 7.21 Thu 17:30 P

Realization of dedicated holder for free standing liquid crystal films: first step towards High Harmonic Generation in Smectic Liquid Crystals — ●KLARA MARIA NEUMANN, PATRICK FRIEBEL, IVAN TRANCART, and LAURA CATTANEO — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg

High harmonic generation (HHG) by a long-wavelength driving field has been recently used as an all-optical probe of the band structure of crystals and liquids (e.g. water) [1,2], showing that the tunneled out electronic wave packet is a sensitive probe of the materials symmetry. This provides an ultrafast all-optical non-invasive probe of the local order in the generating medium. To date, HHG in soft matter samples such as liquid crystals has not been investigated. In this work we present the realization of a holder for free standing liquid crystal films (FSLCF) with controllable thickness and temperature at an accuracy of $\pm 0.1K$ [3]. To form FSLCFs we use 8 CB (4'-n-octyl-4-cyano-biphenyl) liquid crystal, in smectic A phase at room temperature [3]. Thickness measurements are performed using a dedicated autocorrelator setup enabling a thickness control down to few tens of nanometers [4]. The FSLCF will be exposed to strong laser fields in the near infrared ($5\mu m$) to generate High Harmonics in the visible spectrum. [1] Vampa, G. et al. *Nature* **522**, 462-464 (2015); [2] Luu, T.T. et al. *Nature Communications*, **9** (2018); [3] P. L. Poole et al. *Applied Physics Letters* **109**, 151109 (2016); [4] <https://www.brown.edu/research/labs/mittleman/sites/brown.edu.research>

MO 7.22 Thu 17:30 P

Mid-IR Photo-induced Dissociation of Solvated (Bio)Molecular Complexes — ●MUKHTAR SINGH^{1,2,3}, MATTHEW

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We present the ultrafast imaging of thermal-energy chemical dynamics of micro-solvated (bio)molecular complexes when probing with strong-field techniques. We produce a pure sample of the molecule of interest in the gas phase by using a combination of a molecular beam and electrostatic deflector [1]. To study the thermally-induced dynamics, we set up a mid-IR pump-probe experiment, in which a 3 μm beam was used to excite the system and then a 1.3 μm beam was used for ionising the system. First experiments focus on the ion-imaging of the mid-IR pumped system. Future experiments will use laser-induced electron diffraction (LIED) [2,3] to probe the thermally-induced dynamics and obtain structural information about the system with atomic resolution.

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

[2] J. Wiese, et al., *Phys. Rev. Research* **3**, 013089 (2021).

[3] E. T. Karamatskos, et al., *J. Chem. Phys.* **150**, 244301(2019).

MO 7.23 Thu 17:30 P

Time Resolved THz Dynamics in Liquid Crystals — ●PATRICK FRIEBEL, KLARA MARIA NEUMANN, IVAN TRANCART, and LAURA CATTANEO — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

Beyond the typical solid, liquid, and gaseous states of matter, certain materials exhibit mesophase properties, combining attributes of those categories. Liquid crystals (LCs), as a common example, show both solid-like order and fluid-like flow. So far, dynamics occurring within picosecond timescales in LCs are largely unexplored. They show resonant features in the THz spectral region [1], but a clear understanding of these signatures has yet to be developed. Here, we use few cycle THz pulses, generated via optical rectification in the organic crystal DSTMS, to perform both time-domain spectroscopy and resonant time-resolved birefringence measurements on various members of the nCB family of liquid crystals. The measured absorption spectra for uniformly aligned 5CB and 8CB, presenting nematic and smectic A phase, respectively, clearly indicate activity in the THz region. The THz induced birefringence associated with this activity shows oscillatory behaviour after the exciting pulse and thermalization within a few picoseconds. Our time resolved investigation includes dependences on THz-field strength, pump and probe polarization independently controlled with respect to the LC alignment, and temperature, covering phase transitions. Interpretation and attribution to intra- or inter-molecular origin of the data is supported by gas phase theoretical calculations. [1] Vieweg, N., et al., *Optics Express*, 2012. 20(27)

MO 7.24 Thu 17:30 P

Observation of long-lived electronic coherences at room temperature in lanthanide-complexes — ●MIRALI GHEIBI, JAYANTA GHOSH, CRISTIAN SARPE, BASTIAN ZIELINSKI, TILLMANN KALAS, ELENA RAMELA CIOBOTEA, ARNE SENFTLEBEN, THOMAS BAUMERT, and HENDRIKE BRAUN — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The aim of SMolBits - Scalable Molecular Quantum Bits - is the realization of ideal quantum systems with long-lived levels, isolated from the environment to form quantum bits as key building blocks for advanced quantum technologies. Lanthanides are particularly promising with respect to possible applications in quantum-based information storage because their energy levels and electronic states are barely influenced by the environment and bonds to ligands attached to the lanthanides. We are investigating the electronic coherences resonantly excited in lanthanide complexes by interaction with IR femtosecond laser pulses and their lifetimes using phase-locked double pulses and fluorescence detection under a confocal microscope. We observe an electronic coherence time of more than 600 fs for three different complexes containing Neodymium for the excitation from its ground state $^4I_{9/2}$ to the states $^4F_{5/2}$ and $^2H_{9/2}$. Furthermore, characteristics of the electronic wave packet created in the excited states are imprinted onto the coherences. This signal can be observed as a slowly decaying Rabi oscillations in these complexes. As a next step we will investigate the influence of spectrally phase shaped femtosecond laser pulses in the non-perturbative regime onto the electronic excitation and the created coherence.