Molecular Physics Division
Fachverband Molekülphysik (MO)

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Overview of Invited Talks and Sessions

(Lecture halls P 105, P 110, and P 204; Poster Philo 1. OG)

Invited Talks

MO 1.1	Mon	11:30–12:00	P 105	**Unraveling the early-stage dynamics of ionized water dimer in energy and time** — •Sebastian Trippel, Ivo Vinklárek, Michal Belina, Luisa Blum, Hubertus Bromberger, Petr Slavíček, Jochen Küpper
MO 2.1	Mon	11:30–12:00	P 110	**Charge-directed reactivity in chiral molecules induced by ultrafast co-rotating currents** — •Aurelien Sanchez, Erik Månsson, Vincent Wanie, Olga Smirnova, Valerie Blanchet, Yann Mairesse, Bernard Pons, Francesca Calegari
MO 2.2	Mon	12:00–12:30	P 110	**Controlling the orientational degeneracy of rotational states in chiral molecules** — •Elahe Abdiha, Shilpa Yadav, Sejun An, JuHyeon Lee, Boris G. Sartakov, Gerard Meijer, Sandra Eibenberger-Arias
MO 4.1	Mon	17:00–17:30	P 105	**A two-color glimpse at nanomatter: ultrafast movies coming soon.** — •Alessandro Colombo, Linos Hecht, Daniela Rupp
MO 5.1	Mon	17:00–17:30	P 204	**Charge migration in aromatic amino acids** — •Sabine Rockenstein
MO 8.1	Tue	11:00–11:30	P 105	**Observation of diffraction oscillations and low-energy resonances in elastic collisions between He Rydberg atoms and HD molecules** — •Arijit Das, Yufeng Wang, Karl Horn, Piotr Zuchowski, Julia Narevicius, Edvardas Narevicius
MO 9.1	Tue	11:00–11:30	P 110	**All-Optical Enantiomeric Conversion Observed in a Femtosecond Molecular Movie** — •Nicolas Ladda, Fabian Westmeier, Tonio Rosen, Sudheendran Vasudevan, Simon Ranecky, Sagnik Das, Krishna Singh, Hendrike Braun, Jochen Mikosch, Thomas Baumert, Arne Senftleben
MO 23.1	Thu	11:00–11:30	P 110	**Large circular dichroism in the total photoemission yield of free chiral nanoparticles created by a pure electric dipole effect** — •Sebastian Hartweg, Dušan K. Božanić, Gustavo A. Garcia-Macias, Laurent Nahon
MO 24.1	Thu	11:00–11:30	P 204	**Electronic Spectra of Doped Diamondoid Cations** — •Parker Crandall, Ronja Schramm, Sebastian Völz, Domenik Schleier, Otto Dopfer
MO 26.1	Thu	14:30–15:00	P 110	**Differentiating Between Enantiomers with Nuclear Quadrupole Coupling Using Microwave Three-Wave Mixing** — •Freya E. L. Berggötz, Monika Leibscher, Wenhao Sun, Christiane P. Koch, Melanie Schnell
MO 29.1	Thu	15:15–15:45	P 105	**Charge and electronics in molecule activation by transition metal clusters** — •Gereon Niedner-SChatteburg, Nils Wolfgramm, Christoph van Wüllen
MO 32.1	Fri	11:00–11:30	P 204	**Time-resolved photoelectron spectroscopy of polycyclic hydrocarbons in rare-gas clusters** — •Leonie Werner, Ulrich Bangert, Sebastian Hartweg, Yilin Li, Arne Morlok, Felix Riedel, Frank Stienkemeier, Lukas Bruder

Invited Talks of the joint Symposium SAMOP Dissertation Prize 2026 (SYAD)

See SYAD for the full program of the symposium.

SYAD 1.1	Mon	14:30–15:00	RW 1	**What graphs can tell us about quantum information** — •Kiara Hansenne
SYAD 1.2	Mon	15:00–15:30	RW 1	**Realization of alkaline-earth circular Rydberg qubits in optical tweezer arrays** — •Christian Hölzl
SYAD 1.3	Mon	15:30–16:00	RW 1	**Pattern Formation and Supersolid-like Sound Modes in a Driven Superfluid** — •Nikolas Liebster
SYAD 1.4	Mon	16:00–16:30	RW 1	**Harnessing time-frequency qudits using integrated nonlinear processes** — •Laura Serino

Invited Talks of the joint Symposium Spin-Boson Models (SYSB)

See SYSB for the full program of the symposium.

SYSB 1.1	Tue	11:00–11:30	RW 1	**Tailoring the quantum dynamics of spins with bosonic baths** — •Giovanna Morigi
SYSB 1.2	Tue	11:30–12:00	RW 1	**Spins, Qubits, and Bosons** — •Guido Burkard
SYSB 1.3	Tue	12:00–12:30	RW 1	**Spin-boson models under strong ac-driving** — •Milena Grifoni
SYSB 1.4	Tue	12:30–13:00	RW 1	**Kibble-Zurek scenario for melting of discrete time crystals** — •Phatthamon Kongkhambut, Hans Kessler, Roy D. Jara Jr., Jayson G. Cosme, Andreas Hemmerich

Invited Talks of the joint Symposium Selected Highlights of AMOP in Austria (SYAU)

See SYAU for the full program of the symposium.

SYAU 1.2	Wed	11:15–11:45	RW 1	**Supersolidity: When Superfluid Flow Meets Crystalline Order** — •Francesca Ferlaino
SYAU 1.3	Wed	11:45–12:15	RW 1	**Charged Helium Nanodroplets: A Cold Laboratory for Molecular Ions** — •Elisabeth Gruber
SYAU 1.4	Wed	12:15–12:45	RW 1	**Advances in Broadband Saturation Spectroscopy: Towards Probing New Physics in the Mid-Infrared** — •Oliver Heckl
SYAU 1.5	Wed	12:45–13:15	RW 1	**Precision laser spectroscopy of the Thorium-229 nuclear transition** — •Thorsten Schumm

Invited Talks of the joint Symposium Light and Chirality: From Fundamentals to Applications (SYLC)

See SYLC for the full program of the symposium.

SYLC 1.1	Wed	14:30–15:00	RW 1	**Enantio-sensitive molecular compass** — P. M. Flores, S. Carlstroem, S. Patchkovskii, M. Ivanov, V. Mujica, A. F. Ordonez, •O. Smirnova
SYLC 1.2	Wed	15:00–15:30	RW 1	**Conjugation, chirality and optical activity** — •Matthew Fuchter
SYLC 1.3	Wed	15:30–16:00	RW 1	**Gas-phase spectroscopy of chiral molecules** — •Anne Zehnacker, Etienne Rouquet, Valéria Lepère, Gustavo Garcia, Laurent Nahon
SYLC 1.4	Wed	16:00–16:30	RW 1	**Toward a low-energy test of the parity symmetry via precise mid-IR spectroscopy of cold chiral molecules** — Agathe Bonifacio, Sahil Viel, Raphaël Hahn, Minh Nhut Ngo, Marylise Saffre, Yuhao Liu, Wenling Dong, Etienne Cantin, Olivier Lopez, Anne Amy-Klein, Mathieu Manceau, •Benoît Darquié

Invited Talks of the joint Symposium Interactions with Negatively Charged Molecules (SYIN)

See SYIN for the full program of the symposium.

SYIN 1.1	Thu	11:00–11:30	RW 1	**Negative ion studies at ISOLDE: from radioactive atoms to molecules** — •Jessica Warbinek
SYIN 1.2	Thu	11:30–12:00	RW 1	**Leak-out spectroscopy in cryogenic ion traps** — •Stephan Schlemmer, Oskar Asvany, Sven Thorwirth, Philipp Schmid, Weslley Silva, Thomas Salomon
SYIN 1.3	Thu	12:00–12:30	RW 1	**Studies of negative ions in a cryogenic storage ring using laser driven state manipulation** — •Dag Hanstorp

SYIN 1.4	Thu	12:30–13:00	RW 1	**Photodetachment spectroscopy and reactions of negative molecular ions** — •Roland Wester

Invited Talks of the joint Symposium Tests of Fundamental Physics with AMO Systems (SYFP)

See SYFP for the full program of the symposium.

SYFP 1.1	Fri	11:00–11:30	RW 1	**Searches for new bosons with isotope shift spectroscopy and the thorium nuclear transition** — •Elina Fuchs
SYFP 1.2	Fri	11:30–12:00	RW 1	**Precision spectroscopy of muonic atoms** — •Randolf Pohl
SYFP 1.3	Fri	12:00–12:30	RW 1	**Quantum-Controlled Molecules for Fundamental Physics and Quantum Science** — •Nicholas Hutzler
SYFP 1.4	Fri	12:30–13:00	RW 1	**Testing Baryon Asymmetry with Antiprotons** — •Stefan Ulmer

Sessions

MO 1.1–1.6	Mon	11:30–13:15	P 105	**Ultrafast Structural Dynamics**
MO 2.1–2.4	Mon	11:30–13:00	P 110	**Chirality I**
MO 3.1–3.5	Mon	11:45–13:00	N 2	**Collisions, Scattering and Correlation Phenomena I (joint session A/MO)**
MO 4.1–4.7	Mon	17:00–19:00	P 105	**Novel Experimental Approaches and Novel Theoretical and Computational Approaches**
MO 5.1–5.6	Mon	17:00–18:45	P 204	**Ultrafast Electronic Dynamics**
MO 6.1–6.6	Mon	17:00–18:45	N 1	**Attosecond physics I (joint session A/MO)**
MO 7.1–7.8	Mon	17:00–19:00	N 2	**Collisions, Scattering and Correlation Phenomena II (joint session A/MO)**
MO 8.1–8.8	Tue	11:00–13:15	P 105	**Cold Molecules (joint session MO/Q)**
MO 9.1–9.7	Tue	11:00–13:00	P 110	**Chirality II**
MO 10.1–10.5	Tue	17:00–19:00	Philo 1. OG	**Poster – Ultrafast Structural Dynamics**
MO 11.1–11.9	Tue	17:00–19:00	Philo 1. OG	**Poster – Chirality**
MO 12.1–12.2	Tue	17:00–19:00	Philo 1. OG	**Poster – Novel Experimental Approaches and Novel Theoretical and Computational Approaches**
MO 13.1–13.7	Tue	17:00–19:00	Philo 1. OG	**Poster – Ultrafast Electronic Dynamics**
MO 14	Wed	13:30–14:00	P 110	**Members' Assembly**
MO 15.1–15.6	Wed	14:30–16:15	N 2	**Interaction with strong or short laser pulses I (joint session A/MO)**
MO 16.1–16.7	Wed	17:00–19:00	Philo 1. OG	**Poster – Attosecond Physics (joint session A/MO)**
MO 17.1–17.4	Wed	17:00–19:00	Philo 1. OG	**Poster – Interaction with VUV and X-ray Light (joint session A/MO)**
MO 18.1–18.3	Wed	17:00–19:00	Philo 1. OG	**Poster – Interaction with Strong or Short Laser Pulses (joint session A/MO)**
MO 19.1–19.3	Wed	17:00–19:00	Philo 1. OG	**Poster – Contributions to SYLC**
MO 20.1–20.4	Wed	17:00–19:00	Philo 1. OG	**Poster – Molecular Collisions and Kinetics**
MO 21.1–21.8	Wed	17:00–19:00	Philo 1. OG	**Poster – Cluster and Nanoparticles (joint session MO/A)**
MO 22.1–22.5	Wed	17:00–19:00	Philo 1. OG	**Poster – Cold Molecules (joint session MO/Q)**
MO 23.1–23.6	Thu	11:00–12:45	P 110	**Contributions to SYLC I**
MO 24.1–24.6	Thu	11:00–12:45	P 204	**Molecular Spectroscopy I**
MO 25.1–25.3	Thu	14:30–15:15	P 105	**Molecular Collisions and Kinetics**
MO 26.1–26.6	Thu	14:30–16:15	P 110	**Contributions to SYLC II**
MO 27.1–27.8	Thu	14:30–16:30	P 204	**Molecular Spectroscopy II**
MO 28.1–28.7	Thu	14:30–16:30	N 2	**Interaction with VUV and X-ray light I (joint session A/MO)**
MO 29.1–29.5	Thu	15:15–16:45	P 105	**Cluster and Nanoparticles (joint session MO/A)**
MO 30.1–30.22	Thu	17:00–19:00	Philo 1. OG	**Poster – Molecular Spectroscopy**
MO 31.1–31.3	Thu	17:00–19:00	Philo 1. OG	**Poster – Collisions, Scattering and Correlation Phenomena (joint session A/MO)**
MO 32.1–32.7	Fri	11:00–13:00	P 204	**Molecular Spectroscopy III**

Members' Assembly of the Molecular Physics Division

Wednesday 13:30–14:00 P 110

MO 1: Ultrafast Structural Dynamics

Time: Monday 11:30–13:15 Location: P 105

Invited Talk MO 1.1 Mon 11:30 P 105

Unraveling the early-stage dynamics of ionized water dimer in energy and time — ●Sebastian Trippel[1,2], Ivo Vinklárek[1], Michal Belina[3], Luisa Blum[1,2], Hubertus Bromberger[1], Petr Slavíček[2], and Jochen Küpper[1,2] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Department of Physics & Center for Ultrafast Imaging, Universität Hamburg — [3]Department of Physical Chemistry, University of Chemistry and Technology, Prague, the Czech Republic

Radiation chemistry in aqueous systems initiated by ionizing radiation is primarily governed by the ultrafast dynamics of water molecules. The prompt response of the aqueous environment involves the formation of hydrated electrons and proton transfer on femtosecond timescales [1]. We employed a disruptive-probing scheme [2] on a purified ensemble of water dimer to investigate the prompt dynamics after strong-field ionization [3]. Investigating the relation of the hydronium fragment kinetic-energy release with the observed timescales reveals a coupling between proton transfer and fragmentation. With the observation of water-dimer-cation stabilization, this provides new insight into the ultrafast post-ionization dynamics underpinning radiation chemistry in aqueous environments.

[1] Schnorr, Belina, et int (7 authors), Slavíček, Moshammer, *Sci. Adv.* **9**, eadg7864 (2023)

[2] Jochim, DeJesus, Dantus, *Rev. Sci. Instrum.* **93**, 033003 (2022)

[3] Vinklárek, Bromberger, Vadassery, Jin, Küpper, Trippel, *J. Phys. Chem* A **128**, 1593 (2024), arXiv:2308.08006 [physics.atm-clus]

MO 1.2 Mon 12:00 P 105

Influence of the Bridging Length on the Ultrafast Isomerization Dynamics of Bridged Azobenzenes in a Molecular Beam — ●Pascal Pessier[1,2], Maria Hergert[1], Lukas Guhl[1], and Friedrich Temps[1] — [1]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Olshausenstraße 40, 24098 Kiel, Germany — [2]now at Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Bridged azobenzenes have drawn considerable attention in the last decade due to their superior photochemical properties compared to conventional azobenzene (AB). Here, the ultrafast isomerization dynamics of two bridged azobenzenes, -C_2H_2-bridged diazocine (Dz) and -CH_2-bridged diazepine (Dzp), were investigated using time-resolved time-of-flight mass spectrometry, photoelectron imaging and photoionization-photofragmentation spectroscopy aided by quantum chemical calculations.

While Dz was found to isomerize in a concerted fashion ($\tau_1 < 38 \pm 1$ fs), Dzp unfolds first and consecutively isomerizes ($\tau_1 < 38 \pm 7$ fs, $\tau_2 = 680 \pm 96$ fs), linked to the increased ring strain by the shorter bridge. Further, the ultrafast unfolding motion (τ_1) enables additional adiabatic transitions close to the D_0 minimum with an unfolded structure rather than the FC region in the single-color photoelectron spectra. In the freshly prepared ion, this induced unfolding motion is then conserved as a highly excited butterfly vibration, observable as pronounced oscillation of parent ion yield.

MO 1.3 Mon 12:15 P 105

Interpolating Grid Potential Energy Surfaces with X-MACE — ●Paul Idzko[1], Daniel Bitterlich[2], Julia Westermayr[2], and Daniel Keefer[1] — [1]Max-Planck-Institute for Polymer Research, Mainz, Germany — [2]Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry - Leipzig University, Leipzig, Germany

The dynamics of electronically excited molecules is most accurately calculated by solving the time dependent Schrödinger equation (TDSE) on a grid. This gives access to the full nuclear wavefunction. A major challenge is to ensure high accuracy of the underlying electronic potential energy surfaces (PES). After performing quantum chemistry calculations on a sparse grid, interpolation to a much finer grid - usable in the dynamics simulations - becomes necessary. This especially applies to Conical Intersections, which exhibit cusps that are hard to interpolate *via* mathematical methods. X-MACE was presented as a deep learning architecture built upon the popular MACE program suite, enabling the learning of several electronic states, as well as the nonadiabatic coupling elements between the states. Here, X-MACE will be used to interpolate between the geometries calculated with quantum chemistry in an active learning approach. We investigate the influence of the *chemical* interpolation with X-MACE in contrast to *mathematical* interpolation (e.g. splines, polynomials...) on the quantum dynamic simulations for the system of 2,5-dichlorofuran.

MO 1.4 Mon 12:30 P 105

Resolving Reactive vs. Non-reactive Pathways in Ultrafast Photodissociation via Pulse Engineering — ●Ilia Kichev, Vesna Erić, and Daniel Keefer — Max-Planck Institute for Polymer Research, Ackermannweg 10, 56128 Mainz, Germany

Ultrafast spectroscopy experiments use coherent laser sources to probe dynamics and chemical reactivity in molecular systems. Ultrafast photodissociation dynamics in substituted furan remain contentious, with experiments attributing primary reactivity to competing pathways: reactive ring (**RO**) opening and non-reactive ring puckering (**RP**). Both pathways encounter regions with conical intersections (**CoIns**), which further complicates the task to spectroscopically untangle them. The main hurdle is the fact that the chosen spectroscopic observables from both pathways are intertwined and difficult to separate. Here, we deploy Quantum Optimal Control Theory (**QOCT**) Pulse Engineering to isolate spectroscopic signals from both pathways. First, we tailor in silico optimal laser pulses that selectively drive the system toward one of the desired pathways. Then, the signal is spectrally examined to identify critical frequency/amplitude motifs governing pathway selectivity. This will lead to further understanding in the specifics of the reaction, enabling improved experiments and a deeper understanding of the dynamics of similar systems.

MO 1.5 Mon 12:45 P 105

Light-induced wave packet dynamics in sulfur dioxide molecules — ●Sanduni Sandeepani Kudagama[1,2], Artem Rudenko[1], and Huynh Van Sa Lam[1] — [1]Kansas State University, Manhattan, KS, USA — [2]EuXFEL, Schenefeld, Germany

With the development of femtosecond lasers and modern imaging techniques, time-resolves studies of ultrafast light-induced dynamics have become an increasingly important topic in molecular physics and photochemistry. To capture ultrafast molecular dynamics in time domain, femtosecond lasers are often used in a pump-probe scheme. In this study, an intense near-infrared (800 nm) or visible (400 nm) pump pulse was used to trigger wave packet dynamics in neutral and singly charged sulfur dioxide, which were then probed by a second, more intense NIR pulse that further ionized and/or dissociate the molecule. The information on the time evolution of the created molecular wave packets were studied employing momentum-resolved ion spectroscopy and channel-selective Fourier analysis on the delay-dependent yield of several singly, doubly, and triply charged final states of the molecule. All channels were dominated by the ionic ground-state bending vibration, whereas the neutral ground-state bending vibration appeared only with the 800 nm pump as a weak signature in several channels. We incorporated inverse Fast Fourier Transform to reveal the initial direction of the wave packet motion in both ionic and neutral ground states. For either pump pulse used, clear signatures of rotational dynamics were observed. Our study also reveals many important quantum mechanical phenomena such as wave packet dephasing and revivals.

MO 1.6 Mon 13:00 P 105

Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes — Somayeh Souri[1], Katrin Winte[1], Daniel Lünemann[1], Daniel Timmer[1], Elena Mena-Osteritz[2], Sergei Tretiak[3], Christoph Lienau[1], and ●Antonietta De Sio[1] — [1]Universität Oldenburg — [2]Universität Ulm — [3]Los Alamos National Laboratory

Non-equilibrium dynamics following photoexcitation in molecular materials arise from a complex interplay of electronic and vibrational motion, with antisymmetric vibrations playing a key role in ultrafast nonadiabatic dynamics, such as at conical intersections. Their direct spectroscopic identification is, however, challenging, since these modes are often Raman inactive and only weakly affect optical transitions. Here, we show experimental signatures of vibronic coupling to antisymmetric modes in the ultrafast symmetry-breaking dynamics of a quasi-quadrupolar dye[1,2] using two-dimensional electronic spectroscopy (2DES). The sub-50-fs 2DES maps reveal an asymmetric peak pattern with characteristic low-energy cross-peaks. We show that these peaks arise from stimulated emission from a double-minimum excited state potential energy surface induced by vibronic coupling to a ~1430 cm-1 antisymmetric mode[2]. Phenomenological essential state model simulations support the results. Our findings show that 2DES with sub-cycle vibrational resolution is a powerful method for identifying antisymmetric modes in the excited state dynamics prior to intramolecular vibrational relaxation and solvation. [1] Winte et al, Nature Chemistry 17, 1742 (2025); [2] Souri et al, submitted (2025)

MO 2: Chirality I

Time: Monday 11:30–13:00 Location: P 110

Invited Talk MO 2.1 Mon 11:30 P 110

Charge-directed reactivity in chiral molecules induced by ultrafast co-rotating currents — •Aurelien Sanchez[1,2,3], Erik Månsson[1], Vincent Wanie[1], Olga Smirnova[4,5], Valerie Blanchet[6], Yann Mairesse[6], Bernard Pons[6], and Francesca Calegari[1,2,3] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Germany — [3]Physics Department, Universität Hamburg, Germany — [4]Max-Born-Institut, Berlin, Germany — [5]Technische Universität Berlin, Germany — [6]Université de Bordeaux - CNRS - CEA, CELIA, France

Geometrical phase effects [1] (or the Berry phase [2]) play crucial roles in chemical reactions [3]. Recently, direct evidence of topological effects has been observed in small, isolated chiral structures [4, 5], supported by theoretical work within the electric dipole approximation [6]. One such technique relies on the ability to control chiroptical properties using broadband, short UV pulses to enhance or suppress the anisotropy parameter of a given molecular enantiomer. Here, we extend this method to measure the forward/backward asymmetry of fragments produced by dissociation following ionisation of the neutral excited parent molecule. In doing so, we obtain clean snapshots of the different ion fragments from a particular molecular enantiomer using velocity map imaging (VMI) in combination with short UV pump pulses (FTL 2.1 fs) and near-infrared circularly polarised light (FTL 4.0 fs). At specific delays, we observe a 20 to 30% asymmetry, thereby demonstrating a method for charge-directed reactivity in chiral molecules.

Invited Talk MO 2.2 Mon 12:00 P 110

Controlling the orientational degeneracy of rotational states in chiral molecules — •Elahe Abdiha, Shilpa Yadav, Sejun An, JuHyeon Lee, Boris G. Sartakov, Gerard Meijer, and Sandra Eibenberger-Arias — Fritz-Haber-Institut der Max-Planck-Gesellschaft; Berlin, 14195, Germany

We present recent experimental advances towards full enantiomer-specific control of the quantum states of chiral molecules using enantiomer-specific state transfer (ESST). Early studies on ESST reported only modest state-specific enantiomeric enrichment, limited to a few percent [1,2]. The main limitations are due to the thermal population of rotational states and their spatial degeneracy. Our group has overcome the limitation due to thermal population and achieved near-complete control of the enantiomers in a triad of rotational states containing the absolute ground state [3]. For this, we developed a new approach combining ultraviolet and microwave radiation to remove population from two out of three rotational states before applying ESST. In our recent work, we address the limitation due to spatial degeneracy when applying ESST to rotational states not including the absolute ground state. Here, M-state dependent Rabi frequencies impede the overall transfer efficiency when employing conventional pulse schemes. We incorporate theoretically tailored pulse schemes [4] and demonstrate enhanced control despite degeneracy. [1] Eibenberger et al. Phys. Rev. Lett. 118, 123002 (2017) [2] Pérez et al. Angew. Chem. Int. Ed. 56, 12512 (2017) [3] Lee et al. Nat. Commun. 15, 7441 (2024) [4] Leibscher et al. Commun. Phys. 5, 110 (2022).

MO 2.3 Mon 12:30 P 110

Bottom-up Analysis of Ro-Vibrational Helical Dichroism — •Mateja Hrast, Georgios M. Koutentakis, Mikhail Maslov, and Mikhail Lemeshko — Institute of Science and Technology Austria, Klosterneuburg, Austria

Helical dichroism (HD) is a proposed method for the resolution of molecular chirality, employing the orbital angular momentum (OAM) of light and hypothesized to arise from electric-dipole-electric-quadrupole interactions. Going beyond the conventional assumptions, we propose a general theoretical framework for the analysis of HD, based on molecular symmetries and rotational eigenstates. Using our recently developed model of molecule-light interaction Hamiltonian we establishing an explicit link between chiral resolution and orbital angular momentum (OAM) exchange in light-matter interaction. Tracing microscopic mechanisms of the OAM transfer, we derive the rotational selection rules, which clearly establish that HD emerges only from the spin-orbit coupling of light, even for beams without the far-field OAM. Our findings refine the conditions for observing HD, provide a tool to re-examine the outcome of prior experiments, and guide future designs for chiral sensing with structured light.

MO 2.4 Mon 12:45 P 110

Geometric mechanisms enabling photoelectron spin and molecular chirality coupling in photoionization — •Philip Caesar Flores[1], Stefanos Carlstroem[1], Serguei Patchkovskii[1], Misha Ivanov[1,2,3], Vladimiro Mujica[4], Andres Ordonez[1,5,6], and Olga Smirnova[1,3,7] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [2]Insitute of Physics, Humboldt University zu Berlin, Berlin 12489, Germany — [3]Technion - Israel Institute of Technology, Haifa, Israel — [4]School of Molecular Sciences, Arizona State University, Tempe, AZ 85287-1604, USA — [5]Department of Physics, Imperial College London, SW7 2BW London, United Kingdom — [6]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany — [7]echnische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

We examine the simplest yet ubiquitous example of spin-chirality coupling: spin-resolved photoionization of randomly oriented chiral molecules, and uncover two universal geometric mechanisms of spin-selective photodynamics, arising solely from electric-dipole interactions and previously unrecognized. These mechanisms are quantified by two pseudovectors stemming from the geometric properties of photoionization dipoles in spin space and in real space. The developed theoretical framework enables rigorous quantification of ‘locking’ between the cation orientation and photoelectron spin, as well the the photoelectron current and its spin. The former effect captures the core of chirality-induced spin selectivity while the latter captures the dynamical origin of spin- and enantio-sensitive multipolar photoelectron currents.

MO 3: Collisions, Scattering and Correlation Phenomena I (joint session A/MO)

Time: Monday 11:45–13:00 Location: N 2

MO 3.1 Mon 11:45 N 2

Floquet Resonances in Ultracold Gas Scattering — •Sebastian Eggert, Axel Pelster, and Christoph Dauer — University of Kaiserslautern-Landau (RPTU)

An alternative mechanism of tuning interactions between cold atoms is proposed, which is based on dynamically creating ”Floquet bound states” using time-periodic fields. By developing a Floquet-scattering theory we show that sharp Floquet resonances occur at which the effective interaction can be tuned to very large attractive or repulsive values. The resulting predictions explain recent experimental data and provide additional tuning possibilities. Analytic predictions are given for adjusting amplitude, frequency and mean of the applied oscillating field in order to to accurately choose location and width of scattering resonances over a wide range. This paves the road to a versatile toolbox of tailored interactions in setups with multiple species.

MO 3.2 Mon 12:00 N 2

Light scattering experiments in dense dipolar gases — •Ishan Varma, Marvin Proske, Rhutwik Sriranga, Dimitra Cristea, and Patrick Windpassinger — Staudingerweg 7, Institute of Physics, JGU Mainz

In ultracold atomic ensembles where interatomic spacing is smaller than the wavelength of scattered light, direct matter-matter coupling through electric and magnetic interactions significantly influence system dynamics, challenging the approximation of atoms as independent emitters. We study the role of magnetic dipole-dipole interactions (DDI) in the cooperative behavior of atomic ensembles using dysprosium, which has the highest ground-state magnetic moment (10 Bohr magnetons).

This talk focusses on the recently performed light scattering experiments in moderately-dense samples of ultracold dysprosium atoms. We study the scattering properties of the sample with respect to frequency detuning from resonance, optical depth, and external magnetic field. A detailed analysis of the fluorescence signal reveals first indications of super- and sub-radiance, which suggest cooperative behavior in the system. In addition, we also discuss the impact of optical dipole trap polarization on atomic lifetime and highlight the recent technical advancements made in vacuum technology and the design of microscope objectives. These developments enable a higher degree of control and accessibility of the atomic sample.

MO 3.3 Mon 12:15 N 2

Transport resonances through periodically driven, weakly coupled impurity — •Jan Mathis Giesen, Daniel Weber, and Sebastian Eggert — Physics Department and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

We consider transport in an optical lattice through quantum well with time periodic driving and apply Floquet theory to calculate tunneling amplitudes. An analytic non-equilibrium solution of the problem is developed which allows the analytic prediction and analysis of the tunneling amplitudes as a function of frequency, driving amplitude, and energy level of the well. One main result is the discovery of a previously unknown resonant switching effect, where a very small driving field can induce perfect transmission. The results are relevant for corresponding setups using ultra-cold gases in optical lattices, photonic waveguides, quantum dots coupled to metallic leads or magnonic systems.

MO 3.4 Mon 12:30 N 2

The interplay between single- and two-body interference of photoelectrons — •Fabian Rohrbach[1], Andreas Buchleitner[1,2], and Christoph Dittel[1,2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

We clarify under which conditions fermionic exchange (anti-) symmetry manifests in the energy spectrum of photoelectrons generated by pulsed light interacting with matter, and how such signature can be discriminated against anticorrelations potentially arising from Coulomb repulsion. We demonstrate that photoelectrons emitted from two metal needle tips exhibit pronounced two-body interference fringes, and analyze how these features interplay with interference on the single-electron level, along different pathways in a pump–probe ionization scheme.

MO 3.5 Mon 12:45 N 2

Protected quantum gates using qubit doublons in dynamical optical lattices — •Lars Fischer, Yann Kiefer, Zijie Zhu, Samuel Jele, Marius Gächter, Giacomo Bisson, Konrad Viebahn, and Tilman Esslinger — Institute for Quantum Electronics & Quantum Center, ETH Zürich, Otto-Stern-Weg 1, 8093 Zürich

Scalable quantum computation relies on configurable qubit connectivity through system-wide, error-free transport of quantum states. Neutral atoms in optical lattices represent a promising platform for quantum computing, where collisional gates provide a controlled mechanism for quantum logic. Here, we present a purely geometric two-qubit SWAP gate that transiently populates qubit doublon states of fermionic atoms in a dynamical optical lattice. Using atomic spin singlets of fermionic potassium-40, we demonstrate the experimental realisation of this quantum holonomy enabled by doublon states. The gate mechanism is based on a geometric evolution in which dynamical phases are entirely absent, making the mechanism intrinsically robust against fluctuations and inhomogeneities in the confining potentials.

We report a loss-corrected two-qubit SWAP gate fidelity of 99.91(7)%, measured across an ensemble of more than 17,000 atom pairs. Combined with tunable atomic collisions, we realise a universal set of two-qubit gates, paving the way toward large-scale, highly connected quantum processors. Our scheme, based on topological pumping of atoms, establishes the foundation for a fault-tolerant computational platform.

MO 4: Novel Experimental Approaches and Novel Theoretical and Computational Approaches

Time: Monday 17:00–19:00 Location: P 105

Invited Talk MO 4.1 Mon 17:00 P 105

A two-color glimpse at nanomatter: ultrafast movies coming soon. — •Alessandro Colombo, Linos Hecht, and Daniela Rupp for the TwoColorCDI-Collaboration — ETH Zurich, Switzerland

Pairs of ultrashort, ultrabright X-ray pulses of distinct wavelengths can now be produced by X-ray Free Electron Lasers (XFELs) [1]. The possibility of precisely controlling their time delay down to the femtosecond regime allows for probing the same system at two different points in time, even down to the natural timescales of electron dynamics. In this talk, we describe how two-color pulses can be combined with diffraction imaging experiments [2], to capture two time-delayed snapshots of a sample and track its light-induced ultrafast changes. In particular, we show results on two-color diffraction patterns acquired at the European XFEL, where two images of the same sample, separated in time by 750 fs, are successfully reconstructed despite the challenging experimental conditions [3]. While improvements on both the instrument and the analysis sides are still necessary to maximize the resolution of the technique, the exciting possibility of two-color diffraction imaging at XFELs, so far considered unviable, opens a new research path for tracking in space and time ultrafast structural and electron dynamics in nanomatter. The long-standing dream of capturing ultrafast movies of nanomatter with an XFEL is finally at hand, along with a new class of experiments yet to be explored.

[1] S. Serkez et al., *Applied Sciences 10, 2728* (2020)

[2] L. Hecht et al., *arXiv:2508.19991* (2025), in review at *Nat Commun*

[3] L. Hecht et al., *arXiv:2508.20153* (2025), in review at *Nat Commun*

MO 4.2 Mon 17:30 P 105

Generation of controlled, dense and shock-frozen protein beams — •Jingxuan He[1,2,3], Lena Worbs[1,2], Surya Kiran Peravali[1,4], Armando D. Estillore[1], Amit K. Samanta[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany — [4]Fakultät für Maschinenbau, Helmut-Schmidt-Universität,Germany

Single-particle x-ray diffractive imaging (SPI) is a powerful method for probing the structures of gas-phase nanoparticles [1]. Despite the successes in artificial nanoparticles [2] and large viruses [3], its application to proteins remains challenging due to low hit rates, weak scattering, and structural instability. Here, we present a buffer-gas-cell-aerodynamic-lens-stack (BGC-ALS) that is capable of producing shock-frozen and focused protein beams. This approach delivers a large number of hydrated proteins into the tiny x-ray focus, making their native-like structures more likely to be probed. Using strong-field ionization with a velocity-map-imaging spectrometer, we characterized the BGC-ALS and demonstrated its applicability to a broad range of macromolecules including proteins. Such protein beams are promising not only for structural determiniation using SPI but also for pump-probe experiments on protein dynamics.

[1] Barty et al. *Annu. Rev. Phys. Chem.* **9**, 415-435 (2013)
[2] Ayyer et al. *Optica* **8**, 15 (2020)
[3] Seibert et al. *Nature* **470**, 78-81 (2011)

MO 4.3 Mon 17:45 P 105

Laser-induced alignment of macromolecules and nanoparticles — •Lukas Vincent Haas[1,2,3], Xuemei Cheng[1], Muhamed Amin[1], Amit Kumar Samanta[1,2,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Department of Physics, Universität Hamburg — [3]Center for Ultrafast Imaging, Universität Hamburg

X-ray free-electron lasers (XFELs) promise to enable the diffractive imaging of single molecules and nanoparticles, but image reconstruction remains a major bottleneck in achieving atomic spatial resolution [1]. Laser-induced alignment of nanoparticles and macromolecules during the diffractive imaging process has the potential to push resolution toward the atomic scale [2].

We present the quantitative computational modeling of nanoparticle alignment using classical mechanics and electrodynamics [3] along with the first experimental evidence of laser-induced alignment of tobacco mosaic virus (TMV) in an XFEL-compatible setup. The alignment was probed through optical scattering. A recently conducted XFEL experiment provides initial results on diffractive imaging of laser-aligned TMV. Comparing computational and experimental results, we conclude that a high degree of alignment is achieved for TMV in our experiments.

[1] K. Ayyer, *et al.*, *Optica* **8(1)**, 15-23 (2021)
[2] J.C.H. Spence, *et al.*, *Phys. Rev. Lett.* **92**, 198102 (2004)
[3] M. Amin, *et al.*, *J. Am. Chem. Soc.* **147(9)**, 7445 (2025)

MO 4.4 Mon 18:00 P 105

Quantum dynamical properties of Oligocene: from Spectroscopy to Machine Learning — •Viktoria Chatrchyan[1], Fabian Jester[2], Maximilian E. Schommer[1], Philipp Kollenz[1], Oskar Kefer[1], Pavel V. Kolesnichenko[1], Jan Freudenberg[2], Uwe H. F. Bunz[2], and Tiago Buckup[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany — [2]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

Femtosecond transient absorption spectroscopy is a powerful technique for probing ultrafast molecular dynamics. However, interpreting the resulting data typically demands extensive human and computational effort to support theoretical models. To address this challenge, we developed a deep neural network capable of real-time analysis of experimental data, enhanced by quantum-mechanical descriptors, to predict the relaxation kinetics of organic chromophores with over 80% accuracy. Evaluation of the neural network on simulated data confirmed the significant improvement of prediction accuracy (6-8%), underscoring the value of hybrid data integration. This model was applied to transient absorption measurements of recently developed oligoacenes due to their intriguing photodimerization properties. The results showed a non-trivial dependence of the multi-step photodimerization efficiency on the number of aromatic rings. The analysis suggests a complicated relationship between formation yield and the stability of the side products for different molecular sizes.

MO 4.5 Mon 18:15 P 105

Novel 340kW continuous-wave enhancement cavity — •Andriana Tsikritea — Department of Physics, TU Dortmund University, 44227, Dortmund, Germany

The design and development of a novel Fabry-Pérot enhancement cavity will be discussed. Using a 43 W continuous-wave input laser at 1064 nm, we report intracavity circulating powers greater than 340 kW and peak laser intensities of 8.7 GW/cm2. Implementing a fast switching scheme, the high-power laser is allowed to circulate the enhancement cavity for specified time durations, spanning 100 μs to 100 ms. The low duty cycle of the switching scheme allows the minimisation of heating effects on the cavity optical components, while simultaneously offering stable and repeatable pulses of the high-power laser.

The enhancement cavity is currently being integrated with a moving magnetic decelerator and superconductive trap apparatus. The high intracavity laser intensity will be used to optically trap polarisable molecular species. For example, for O2 molecules, the reported 340 kW laser power generates a 200 mK deep optical trapping potential. Subsequently, the evaporative cooling of the molecular ensemble will be attempted. With no laser cooling scheme implemented, the optical trapping experiments enabled by the enhancement cavity pave the way for the generation of laser-cooling-free quantum degenerate molecular gases.

MO 4.6 Mon 18:30 P 105

Generation of broad-bandwidth deep ultraviolet pulses using achromatic second harmonic generation — •Nils-Oliver Schütz, Mario Niebuhr, Ulrich Bangert, Felix Selz, Felix Riedel, and Lukas Bruder — Hermann-Herder-Straße 3, 79104 Freiburg, Germany

The generation of deep ultraviolet optical pulses featuring broad spectral bandwidth and short pulse durations is a challenging task, especially when using high repetition rate ($>$ 100kHz) laser systems that provide low pulse energies to drive the nonlinear conversion processes. We present a scheme based on second harmonic generation of the output of a non-collinear optical parametric amplifier. To increase the bandwidth and efficiency of the second harmonic generation we employ achromatic phase matching [1]. Through ray-tracing simulations, the impact of different geometrical arrangements of the setup on the compression of the UV pulses was investigated. The results, together with the characterization of the UV pulses, are presented.

MO 4.7 Mon 18:45 P 105

Facile production of multiply-charged actinide molecules — •J. Stricker[1,2,3], K. Gaul[1,2], P. Fischer[4], D. Renisch[1,2], D. Budker[1,2,3], F. Schmidt-Kaler[1,2,3], L. von der Wense[1], L. Schweikhard[4], and Ch. E. Düllmann[1,2,3,5] — [1]JGU Mainz — [2]HI Mainz — [3]PRISMA+ Mainz — [4]Universität Greifswald — [5]GSI Darmstadt

We present a new method for producing multiply-charged actinide molecules. Using pulsed laser ablation of micro-targets, we generate ThF$_x^{n+}$ (x = 0-3, n $\leq$ 3) from ThF$_4$ salt, and UO^{n+} from metallic uranium up to UO^{4+}. The production of ThF^{2+} and UO^{3+} is particularly relevant for searches for nuclear Schiff moments, while UO^{4+} approaches the limit of chemical stability. Relativistic density-functional calculations validate the observed charge states and molecular structures. The technique provides access to a broad range of multiply-charged radioactive molecules for a variety of future precision experiments.

MO 5: Ultrafast Electronic Dynamics

Time: Monday 17:00–18:45 Location: P 204

Invited Talk MO 5.1 Mon 17:00 P 204

Charge migration in aromatic amino acids — •Sabine Rockenstein for the AMINO-Collaboration — Deutsches Elektronen-Synchrotron DESY

Aromatic amino acids play pivotal roles in protein structure and function. Their prompt ionization can trigger an ultrafast charge motion between the various functional groups. At the Linac Coherent Light Source (LCLS), the enhanced self-amplified spontaneous emission (eSASE, XLEAP) configuration allows attosecond-resolved x-ray absorption spectroscopy of such processes with unprecedented time resolution. Site-specific measurements in a $\omega/2\omega$ XLEAP scheme at the oxygen and nitrogen K edge, exploiting the high data rate available from LCLSII, enable studies of electronic dynamics and electron-nuclear coupling. This technique has been applied to phenylalanine and tryptophan, which, in previous studies with table-top attosecond sources, showed remarkably different dephasing times despite structural similarity. We discuss the experimental methods and the preliminary analysis of the collected data.

MO 5.2 Mon 17:30 P 204

Ultrafast charge transfer dynamics in phosphorylated amino acids in aqueous solution — •Nicolas Velasquez[1], Juliette

Leroux[2], and Florian Trinter[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6 14195, Berlin, Germany — [2]Department of Physics, Universität Hamburg, 22607 Hamburg, Germany

Charge transfer (CT) plays a fundamental role in chemistry and biology, particularly in aqueous environments where most reactions occur. Post-translational modifications such as phosphorylation strongly alter local charge distribution and intermolecular interactions in proteins. In this study, we employ Auger–Meitner spectroscopy to address ultrafast CT dynamics in phosphorylated amino acids in aqueous solution, focusing on the role of the phosphate group at the biomolecule–water interface. Our results indicate that the phosphate group dramatically enhances charge transfer to the solvent (CTTS). This finding highlights the role of solvation and, in particular, hydrogen-bond network effects in facilitating CTTS. Furthermore, the core-hole lifetime provides a natural timescale for electron dynamics, allowing quantification of CT rates. Our observations suggest that CT pathways are governed by the interplay between the phosphate moiety and the amino-acid backbone in the hydrated environment. Understanding CT in biomolecules is crucial for fields such as radiation chemistry, protein chemistry, and biophysics. Our findings contribute to a deeper understanding of early electronic processes in complex systems, paving the way for future studies of radiation-induced damage in biologically relevant conditions.

MO 5.3 Mon 17:45 P 204

Low dispersion, phase-modulated rapid-scanning interferometry in the deep UV spectral region — •Felix Selz, Ulrich Bangert, Fabian Richter, Felix Riedel, Nils-Oliver Schütz, and Lukas Bruder — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Stable interferometer schemes for the deep UV spectral region and ultrashort pulse applications remain limited. Conventional spectrometers typically lack the required phase stability, whereas common-path interferometers introduce substantial temporal dispersion. We have recently developed a low-dispersion interferometric approach that combines high phase stability with excellent sensitivity using an efficient rapid scanning lock-in detection scheme [1]. We are now extending this scheme into the deep UV spectral region with particular emphasis on minimizing material dispersion to ensure compatibility with sub 10-fs laser pulses. This opens up Fourier transform and coherent multidimensional spectroscopy with high temporal and spectral resolution in the deep UV domain.

[1] F. Richter et al., Opt. Lett. 50, 3668-3671 (2025)

MO 5.4 Mon 18:00 P 204

New insight into photoionization by attosecond spectroscopy of isosteric molecules — •Maximilian Pollanka[1], Maximilian Forster[1], Sven-Joachim Paul[1], Zdenek Masin[2], Jakub Benda[2], and Reinhard Kienberger[1] — [1]School of Natural Sciences, Chair for Laser- and X-ray physics, Technische Universität München, Garching, Germany — [2]Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czechia

Our work addresses time-resolved photoemission in molecules. To this end, the four isosteric di-and tri-atomic molecules CO, N2, CO2, and N2O are investigated in complementary studies and compared with each other. By using suitable chronoscopes in combination with the attosecond streaking spectroscopy method, it is possible not only to determine relative photoemission times between different electronic states but also to access absolute photoemission delays. Together with theoretical considerations and simulations, the experimentally obtained results can be discussed and explained. This measurement method is applied to four molecules that are almost identical in their electronic states, molecular orbitals, and number of outer valence electrons, which is described by the term isosterism. The chronoscopes iodomethane (I4d state) and helium (He1s state) are not only used as a reference to gain access to the absolute photoemission times, but the results obtained in separate experiments are also used to verify the validity of the unrestricted use of both. Together with theoretical support, the physical processes underlying photoemission in these isosteric molecules could finally be deciphered and interpreted.

MO 5.5 Mon 18:15 P 204

Investigating higher-excited-state properties through nonlinear order separation in two-dimensional electronic spectroscopy — •Katja Mayershofer[1], Peter A. Rose[2], Julian Lüttig[2], Luisa Brenneis[1], Simon Büttner[1], Jacob J. Krich[2,3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Ottawa, Ottawa, Ontario, Canada — [3]Nexus for Quantum Technologies, University of Ottawa, Ottawa, Ontario, Canada

Recently, we developed an implementation of coherent two-dimensional (2D) electronic spectroscopy that enables us to separate signals of different pertubative orders through intensity variation and inversion with a Vandermonde matrix [1]. We applied this new technique to investigate a squaraine dimer. This procedure allowed us to obtain signals of different nonlinear orders that are uncontaminated from overlapping higher orders. We observe changes in the lineshapes from third to higher orders. To gain further insight into the higher-excited states of our sample, we performed simulations using the Ultrafast Spectroscopy Suite toolbox [2,3]. Through the combination of uncontaminated higher-order 2D signals and simulations, we retrieve transition dipole moments and energy levels of higher-excited states, giving us a new way to verify and improve theoretical models.

[1] J. J. Krich et al., J. Phys. Chem. Lett. **2025**, *16*, 5897.
[2] P. A. Rose & J. J. Krich, J. Chem. Phys **2021**, *154*, 034108.
[3] P. A. Rose & J. J. Krich, J. Chem. Phys **2021**, *154*, 034109.

MO 5.6 Mon 18:30 P 204

Efficient Two-Dimensional Spectroscopy Simulations including Realistic Pulse Shapes, Overlapping, and Time-Ordering Effects — •Rémi Gilliot[1,2], Matteo Russo[1], Alexander Blech[1], Manuel Joffre[2], Christiane Koch[1], and Hélène Seiler[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Institut Polytechnique de Paris, Palaiseau, France

Two-dimensional (2D) spectroscopy is a powerful pump-pump-probe method to reveal coupling between quantum states and disentangle optical response contributions. We present an efficient approach for simulating 2D spectra with arbitrary pulse shapes including overlapping and time-ordering. Under the assumption of simple dephasing, we show that the emitted signal expression reduces to three independent nested integrals, that can be computed in linear time. We utilize this approach to study the impact of spectral phase distortions and strongly non-Gaussian pulse shapes - such as those produced experimentally by hollow-core fibers.

MO 6: Attosecond physics I (joint session A/MO)

Time: Monday 17:00–18:45 Location: N 1

Invited Talk MO 6.1 Mon 17:00 N 1

Measurement of neon photoemission delays and double-core-hole Auger-Meitner lifetime using Angular Streaking — •Lars Funke[1], Sara Savio[1], Lasse Wülfing[1], Niclas Wieland[2], Markus Ilchen[2], and Wolfram Helml[1] — [1]Fakultät Physik, Technische Universität Dortmund, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, Germany

The extreme brightness of X-ray free electron lasers allows probing non-linear processes in atoms and molecules in single-shot measurements. The addition of a temporal reference, e.g. through an Angular Streaking setup, enables the direct measurement of observables previously only accessible indirectly.

Here, we report on a European-XFEL measurement that simultaneously yields relative emission delays for multiple transitions triggered by 990 eV photons in neon. Specifically, we are able to clock 1s, 2s and 2p photoelectrons, single- and double-core-hole Auger-Meitner electrons at the same time, owing to a multi-resolution time-of-flight detector setup covering a broad electron energy range.

MO 6.2 Mon 17:30 N 1

Observation of sub-cycle ponderomotive acceleration via near-field-induced low-energy stripes (NILES) — •L. Seiffert[1], J. Heimerl[2], S. Meier[2], A. Herzig[1], F. Lòpez

Hoffmann[2], D.M.B. Lesko[2], S. Hillmann[2], S. Wittigschlager[2], T. Weitz[2], T. Fennel[1,3], and P. Hommelhoff[2,4] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Physics, Friedrich Alexander University Erlangen-Nuremberg, Germany — [3]Department of Life, Light and Matter, University of Rostock, Germany — [4]Faculty of Physics, Ludwig Maximilian University Munich, Germany

Ponderomotive acceleration of electrons in strong fields is typically regarded as a cylce-averaged effect and hence mostly associated with long pulses. However, recently, subcycle sensitivity of the ponderomotive acceleration effect has been reported for electrons injected into the strong near-field gradient of a sharp metal tip by a few-cycle optical waveform [1]. In this talk the recent observation of this effect which manifests in the direct electrons part of carrier-envelope-phase-dependent electron spectra in the form of near-field-induced low-energy stripes (NILES) will be discussed from a theoretical point of view. These stripes allow the tracking of direct and rescattered electron emissions on subcycle timescales and provide access to the electron momentum width at emission.

[1] J. Heimerl at al., Nat. Phys. (2025)

MO 6.3 Mon 17:45 N 1

A rigorous and universal approach for highly-oscillatory integrals in attosecond science — •Anne Weber[1], Job Feldbrugge[2], and Emilio Pisanty[1] — [1]Attosecond Quantum Physics Laboratory, King's College London, WC2R2LS London, UK — [2]Higgs Centre for Theoretical Physics, University of Edinburgh, UK

Light-matter interactions within the strong-field regime, such as high-harmonic generation, typically give rise to highly-oscillatory integrals, which are often solved using saddle-point methods. Not only do these methods promise a much faster computation, but they also inform a more intuitive understanding of the process in terms of quantum orbits, as the saddle points correspond to interfering quantum trajectories (think Feynman's path integral formalism). Despite these advantages, a sound understanding of how to apply saddle-point methods to highly-oscillatory integrals in a rigorous way, and with algorithms which work uniformly for arbitrary configurations and laser drivers, remains lacking. This hinders our ability to keep up with state-of-the-art experimental setups which increasingly rely on tightly-controlled laser waveforms. Here, I will introduce the key ideas of Picard-Lefschetz theory – the foundation of all saddle-point methods – and their implementation. Using high-harmonic generation and above-threshold ionisation as examples, I will show how those ideas provide a robust framework for the fast computation of integrals, as well as a widely-applicable algorithm to derive the relevant semiclassical quantum orbits that underlie the physical processes.

MO 6.4 Mon 18:00 N 1

Structured light for enhanced attosecond chiral sensing — •Nicola Mayer[1], Anne Weber[1], Daniele Toffoli[2,3], Margarita Khokhlova[1], and Emilio Pisanty[1] — [1]Attosecond Quantum Physics Group, King's College London, London (United Kingdom) — [2]Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli studi di Trieste, Via L. Giorgieri 1, I-34127, Trieste, Italy — [3]IOM-CNR, Istituto Officina dei Materiali, 34149, Trieste, Italy

Chirality is an ubiquitous phenomenon in nature, spanning many orders of magnitude in length, from the cosmic scale in spiraling galaxies to the microscopic one in chiral molecules. The interaction of polychromatic synthetic chiral light beams (SCL) with chiral molecules is expected to enhance chiral signals in observables such as HHG or photoelectron yield. Here, we show that by using vector-vortex beams with radial and azimuthal polarization, the chirality of SCL beams carrying a chiral topological charge can be increased by two orders of magnitude, leading to a huge enhancement in chiral signals. We prove theoretically such enhancement by using an ab-initio based strong-field approximation approach to describe HHG in fenchone and camphor, with state-of-art saddle point methods to describe polychromatic three-dimensional quantum orbits in the continuum. Our results bring the goal of experimental proof of these techniques closer to reach, both in chiral molecules as well as in atoms.

MO 6.5 Mon 18:15 N 1

Absolute photoemission timing in noble gases — •Maximilian Forster[1], Maximilian Pollanka[1], Sven Paul[1], Christian Schröder[1], Pascal Freisinger[1], Anatoli Kheifets[2], and Reinhard Kienberger[1] — [1]Chair for laser and x-ray physics, E11, Technische Universität München, Germany — [2]Research School of Physical Sciences, The Australian National University, Canberra ACT 0200, Australia

We measured the photoemission time delay in noble gases, namely neon and xenon across different photon energies using the attosecond streaking technique.

The photoemission delay of neon, being the first ever evidence of atomic delay, has received repeated attention by both experimental and theoretical investigations due to the large cross section and convenient properties of neon. As a helium reference is no possible for neon, we used iodoemthane as a chronoscope. The internal delay between Ne2s and Ne2p can be extracted simultaneously, allowing for a consistency check with previous experiments conducted only with neon.

The Xenon states Xe4d and Xe5s can be measured straightforward relative to helium and are compared to theoretical calculations.

MO 6.6 Mon 18:30 N 1

Attosecond XUV-XUV Fourier Transform Spectroscopy of Autoionizing Rydberg States in Molecular Nitrogen — •Ignacio Martínez Casasús[1], Oleg Kornilov[2], Arnaud Rouzée[2], Luis Bañares Morcillo[1,3], and Tobias Witting[2] — [1]Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain — [2]Max Born Institute, Max-Born-Straße 2A, 12489 Berlin, Germany — [3]Instituto Madrileño de Estudios Avanzados IMDEA-Nanoscience, Faraday, 9, 28049 Madrid, Spain

We introduce attosecond XUV-XUV Fourier transform spectroscopy to investigate the autoionizing Rydberg states of molecular nitrogen. Phase-locked XUV pulse pairs are generated through high-harmonic generation and delayed with sub-10-attosecond timing precision. The first pulse prepares a coherent superposition between the molecular ground state and a set of high-lying Rydberg states. The second pulse probes the evolving coherence, imprinting delay-dependent modulations onto the population of autoionizing levels. These modulations are subsequently read out via the photoelectron spectra resulting from autoionization into different ionic continua. Fourier analysis of the delay-dependent photoelectron yields provides information about transition energies, coherence dynamics and vibrationally resolved ionization cross-sections.

MO 7: Collisions, Scattering and Correlation Phenomena II (joint session A/MO)

Time: Monday 17:00–19:00 Location: N 2

MO 7.1 Mon 17:00 N 2

Theory of Electronic Transitions — •Hubert Klar — retired from University Freiburg, Institut für Physik — 79000 Freiburg, Hermann-Herder-Strasse 3

Starting from the Hamilton-Jacobi frame we present a novel parabolic partial difference equation for s-wave electron atom scattering.This equation serves for initial value problems.Thanks to an unexpected separation of coordinates we calculate easily the classical action which we use later to derive a quantum wave function in the semiclassical limit including correlation. There is no way for direct excitation. That lack is filled by a correlated multielectron wave propagation along a potential ridge. The final destination of that wave is a multielectron concentration point, i. e. all correlated electrons arrive near the nucleus. In the special case of single excitation two electrons form a pair comparable to a Cooper pair.These pairs fill a lake whose elements are represented by converging and diverging Fresnel distributions. The concentration point is highly unstable, the decay leads to an excited target state plus an escaping electron.Our results are in conflict with the old Born model for several reasons. (i) We describe the electrons by matrial waves rather by mass-points. (ii) Correlation has been properly takn in account. (iii) The target electron is not kicked up but pulled up due to electron-electron attraction.

MO 7.2 Mon 17:15 N 2

Asymmetries observed in vibrational dissociation of HD by proton impact — •Michael Schulz[1,2], Shruti Majumdar[1], Sujan Bastola[1], Basu Lamicchane[1], Daniel Fischer[1], Ahmad Hasan[3], and Ramaz Lomsadze[4] — [1]Missouri University of Science & Technology, Rolla, USA — [2]Max-Planck Institut für Kernphysik, Heidelberg, Germany — [3]UAE University, Al Ain, UAE — [4]Tbilisi State University, Tbilisi, Georgia

We have measured momentum-analyzed H+ and D+ molecular fragments produced in p + HD collisions in coincidence with neutralized scattering-angle resolved projectiles. From the data we extracted multiple (including fully) differential cross sections for dissociative capture. In various spectra we observed a pronounced asymmetry favoring the H+ + D0 over the H0 +D+ fragmentation channel. A qualitatively similar, but weaker asymmetry was previously found for dissociative ionization and well reproduced by theory [1]. It was explained by an isotope shift in the asymptotic molecular energy curves favoring the electron to be localized closer to the deuteron. We conclude that the same explanation holds for our results on dissociative capture. The larger magnitude of the asymmetry is probably due to the significantly smaller projectile energy.

[1] I. Ben-Itzhak et al., Phys. Rev. Lett. 85, 58 (2000)

MO 7.3 Mon 17:30 N 2

Coherent Ionization of Atoms by Dense and Compact Beams of Extremely Relativistic Electrons — •Sami Kim, Carsten Müller, and Alexander B. Voitkiv — Institut für Theoretische Physik I, Heinrich-Heine-Universität Düsseldorf

Coherent ionization of atoms by very dense and compact beams of highly relativistic electrons is studied [1]. We consider and compare two coherent electron-induced ionization mechanisms, tunnel/over-barrier ionization and coherent impact ionization. In both mechanisms, a significant fraction of the beam electrons acts coherently, leading to a substantial ionization enhancement. The low-frequency components of the total beam field can coherently induce tunneling in target atoms, while the high-frequency components enable coherent impact ionization. The processes are shown to depend very sensitively on the spatiotemporal structure of these novel electron beams, which offers a means for their characterization.

[1] S. Kim, C. Müller and A. B. Voitkiv; arXiv:2508.17192v2

MO 7.4 Mon 17:45 N 2

Detachment with target ionization in collisions of slow D- ions with He and Ar — •Michael Schulz[1], Felix Hermann[1], Weiyu Zhang[1], Alexander Voitkiv[2], Bennaceur Najjari[3], Maka Siddiki[1], Alexander Dorn[1], Manfred Grieser[1], Florian Grussie[1], Holger Kreckel[1], Olda Novotny[1], Andreas Wolf[1], Thomas Pfeifer[1], Claus Dieter Schröter[1], and Robert Moshammer[1] — [1]Max Planck Institut für Kernphysik, Heidelberg, Germany — [2]Heinrich Heine University, Düsseldorf, Germany — [3]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, China

We have measured momentum-analyzed recoil-ions and ejected electrons in triple coincidence with projectiles neutralized in collisions of D- ions with He and Ar at projectile energies between 20 and 120 keV. From the data we extracted multiple-differential momentum distributions of electrons ejected in detachment accompanied by single target ionization. For the Ar target the results confirm a strong role played by a first-order correlated channel proceeding by a mutual interaction between the active projectile- and target- electrons which we observed earlier for Si- projectiles. Surprisingly, this is the case even well below the threshold energy for this mechanism pointing to the significance of the interaction between the two active electrons in this fundamental scattering process. The first-order process is important for the He target as well, however, there signatures of higher-order channels are more pronounced than for Ar. The data are qualitatively well reproduced by our higher-order calculations.

MO 7.5 Mon 18:00 N 2

Rate coefficients for dielectronic recombination of the astrophysically relevant N-like Ne ion at CRYRING@ESR — •Elena-Oana Hanu[1,2,3], Michael Lestinsky[1], Carsten Brandau[1], Michael Fogle[5], Pierre-Michel Hillenbrand[1], Mirko Looshorn[6,7], Esther Menz[1,4], Stefan Schippers[6,7], Reinhold Schuch[8], Maria Tatsch[6,7], Ken Ueberholtz[9], Shu-Xing Wang[6,7], and Thomas Stoehlker[1] — [1]GSI GmbH, Darmstadt — [2]HI Jena — [3]GU Frankfurt am Main — [4]Universität zu Köln — [5]Dep. of Physics, Auburn University, USA — [6]I. Physikalisches Institut, Uni Giessen — [7]HFHF, Giessen — [8]Dep. of Physics, Stockholm University, Sweden — [9]IKP, Uni Muenster

Dielectronic recombination of N-like Ne was studied using a merged-beams setup at CRYRING@ESR for collision energies from 0 to 25 eV. The measured energy-dependent recombination rate coefficient includes all ΔN=0 DR resonances from 2s to 2p core excitations was compared with results from theoretical calculations. The ion beam contained roughly equal fractions of ions in the ground-state and in metastable states, therefore the theoretical rates were weighted accordingly. From the measurements we derived a DR plasma rate coefficient α(T). The results agree well with previous theory for high temperatures where N-like Ne is abundant, but yield slightly higher rates at the lower temperatures typical of photoionized plasmas and collisionally ionized plasmas. Parametrized fits of the experimental DR plasma rates are provided for use in astrophysical models.

MO 7.6 Mon 18:15 N 2

Electron gun optimization for electron-ion crossed-beams experiments — •B. Michel Döhring[1,2], Kurt Huber[1], Mirko Looshorn[1,2], and Stefan Schippers[1,2] — [1]Justus-Liebig-Universität Gießen — [2]Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt

Electron-impact ionization is a fundamental atomic collision process, which is of importance for a wide range of scientific and technical applications such as astrophysics, EUV lithography and fusion research [1]. Recent cross-section measurements with moderately charged xenon ions [2] and singly charged lanthanum ions [3] have demonstrated the excellent performance of our high-current electron gun, which we have designed and built in Giessen [4,5]. This gun has also served as a prototype of the transverse free electron target for CRYRING at GSI/FAIR [6]. Here, we report on our latest achievements in electron beam resolution, on measurements particularly in the low-energy region, and on future plans for optimizing the flexible electron gun.

[1] A. Müller, Adv. At. Mol. Opt. Phys. **55**, 293 (2008).
[2] F. Jin et al., Eur. Phys. J. D **78**, 68 (2024).
[3] B. M. Döhring et al., Atoms **13**, 2 (2025).
[4] W. Shi et al., Nucl. Instrum. Meth. B **205**, 201 (2003).
[5] B. Ebinger et al., Nucl. Instrum. Meth. B **408**, 317 (2017).
[6] M. Lestinsky et al., Eur. Phys. J. ST **225**, 797 (2016).

MO 7.7 Mon 18:30 N 2

A Novel Compton Telescope for Polarimetry in the MeV Range: Towards Delbrück Scattering — •Tobias Over-Winter[1,2,3], Anton Kononov[1], Thomas Krings[4], Wilko Middents[1,2,3], Uwe Spillmann[1], Günter Weber[1,2], and Thomas Stöhlker[1,2,3] — [1]Helmholtz Institute Jena, Jena, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany — [3]Friedrich Schiller University Jena, Jena, Germany — [4]Forschungs Zentrum Jülich, Jülich, Germany

For photon energies from several tens of keV up to a few MeV, Compton polarimetry provides insight into subtle details of fundamental radiative processes in atomic physics. Within the SPARC collaboration [1] several segmented semiconductor detectors have been developed that are well suited for application as efficient Compton polarimeters. For scattering and photon emission processes in the hard x-ray regime this kind of detector enable revealing photon polarization effects in great detail [2]. Recently, a new polarimeter has been constructed within the SPARC collaboration based on an arrangement of two segmented semiconductor crystals in a telescope structure. This design allows us to employ the Compton polarimeter in a broad energy range of photon energies from 50 keV up to 1 MeV. In my contribution I will present this detector. Additionally, I will discuss first planned experiments utilizing this detector at high photon energies up to 1 MeV.

[1] Th. Stöhlker et al. Nucl. Instrum. Methods Phys. Res. B 365 (2015) 680.

[2] K.H. Blumenhagen et al. New J. Phys. 18 (2016) 119601.

MO 7.8 Mon 18:45 N 2

Single-Electron Detection at Room Temperature Using Background-Gas Ion Signals in a Penning Trap — •Arindam

Kumar Sikdar[1,2], Joydip Nandi[1,2], M. Chatterjee[3], Vyshnav C.H.[4], A Ray[1], K. T. Satyajith[4], and P. Das[1,2] — [1]Variable Energy Cyclotron Centre, 1/AF Bidhannagar, Kolkata, INDIA — [2]Homi Bhabha National Institute, Anushaktinagar, Mumbai, Maharashtra, INDIA — [3]Jadavpur University, Raja Subodh Chandra Mallick Road, Jadavpur, Kolkata, INDIA — [4]Delta Q, IMJ Institute of Research, Moodlakatte, Karnataka, INDIA

We present a simple, room-temperature method for detecting a single trapped electron without relying on cryogenic electronics or image-current readout. A single electron confined in a Penning trap naturally ionizes residual background molecules, producing low-energy ions that are guided to a microchannel plate (MCP) and counted individually. These ion bursts provide a clear, indirect signature of the electron*s presence and confinement dynamics.

This ionization-based readout is highly sensitive, non-invasive, and directly compatible with hybrid trap architectures such as dual-frequency Paul traps and Penning*Paul combinations, where conventional detection is limited by weak image currents and RF noise. The technique offers a practical path toward single-lepton detection in room-temperature electron, positron, and antimatter experiments, and opens new opportunities for compact precision sensors and single-particle studies.

MO 8: Cold Molecules (joint session MO/Q)

Time: Tuesday 11:00–13:15 Location: P 105

Invited Talk MO 8.1 Tue 11:00 P 105

Observation of diffraction oscillations and low-energy resonances in elastic collisions between He Rydberg atoms and HD molecules — •Arijit Das[1], Yufeng Wang[1], Karl Horn[1], Piotr Zuchowski[2], Julia Narevicius[1], and Edvardas Narevicius[1] — [1]Technische Universität Dortmund, Dortmund, Germany — [2]Nicolaus Copernicus University, Torun, Poland

Observation of shape and Feshbach resonances in low-energy ion-neutral collisions has been a long-standing goal, but such collisions at cold temperatures remain elusive because of the difficulty of controlling ion beams. While Feshbach resonances between ions and atoms have been observed using magnetically tunable interactions [1], Rydberg atoms offer a powerful platform for exploring quantum collision dynamics in ion-molecule systems. The Rydberg electron acts as a spectator, effectively shielding the ion core and enabling precise investigations of long-range interactions during ion core-molecule collisions.

In this work, we investigate elastic collisions between helium Rydberg atoms and HD molecules at cold temperatures using a merged-molecular-beam apparatus. Velocity-map images of scattered helium reveal pronounced diffraction oscillations linked to partial-wave contributions dominated by ion core-neutral interactions. By tuning the collision energy, we also observe a series of low-energy scattering resonances. These observations provide a new pathway for detecting low-energy ion-molecule resonances that have, until now, remained inaccessible.

(1) Weckesser, Pascal, et al. Nature, 600, 429-433 (2021).

MO 8.2 Tue 11:30 P 105

Surface collision and thermalisation of a laser-coolable molecule aluminium monofluoride — •Pulkit Kukreja, Lasse Rautenberg, Sebastian Kray, Gerard Meijer, and Sid Wright — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Until very recently, direct laser cooling of molecules has been restricted to reactive species with $^2\Sigma$ electronic ground states. These molecules are challenging to produce and have only been captured into a magneto-optical trap (MOT) from pulsed, cryogenically cooled molecular beam sources. These are rather complex, expensive, and difficult to operate reliably for long periods.

At the Fritz Haber Institute, we have now realised the first MOT of a spin-singlet molecule: aluminum monofluoride (AlF). AlF has high chemical stability compared to $^2\Sigma$ molecules, and can also be made efficiently at moderate temperatures (~ 900 K) in an oven. Remarkably, we observe that AlF can survive collisions with, and therefore thermalise to, room temperature vacuum walls of our experiments.

Here, we present the outcomes of single AlF-surface collisions on a camera via Doppler-sensitive laser-induced fluorescence. We observe that AlF undergoes trapping-desorption at surfaces, with complete rovibrational and translational thermalisation to the surface. The collision outcomes are highly surface-dependent, with polydimethylsiloxane (PDMS) coatings having a low sticking coefficient. Our results open a pathway to molecular MOTs loaded from compact and inexpensive beam sources and suggest that the technology employed in atomic vapour cells can be applied to a laser-coolable molecule.

MO 8.3 Tue 11:45 P 105

Decoding Feshbach resonances of Ne+HD+ reaction using ion-electron coincidence and merged beam techniques — •Yufeng Wang[1], Arijit Das[1], Baruch Margulis[2], Karl Horn[1,3], Meenu Upadhyay[4], Markus Meuwly[4], Christiane Koch[3], and Edvardas Narevicius[1] — [1]Technische Universität Dortmund — [2]National Institute of Standards and Technology — [3]Freie Universität Berlin — [4]University of Basel

Feshbach resonance in collisions is an interesting quantum effect. In AMO studies, Feshbach resonance is widely used to produce Feshbach molecules by tuning the magnetic field. In reaction dynamics studies, Feshbach resonances also play a critical role in influencing the scattering cross section. However, this important phenomenon remains unclear to us due to the difficulty of experimental measurement.

Here, we developed a new method to investigate the Feshbach resonance based on ion-electron coincidence measurements, starting with a cold collision that leads to Penning ionization.[1] This new method was applied to research on Feshbach resonances in the Ne and HD+ collision. Assisted by the merged-beam technique, we lowered the collision energy to 22 mK and realized a p-wave (l=1) scattering. Combined with the high-resolution velocity map imaging technique, more substructures were observed and assigned to the Feshbach resonances arising from different vibrational modes of Ne-HD+ by high-accuracy quantum calculations. This work deepens our understanding of the Feshbach resonances in scattering.

(1) Margulis, B. et al. Science 380,77-81(2023).

MO 8.4 Tue 12:00 P 105

Magneto-optical trapping of aluminum monofluoride — •Jionghao Cai[1], José Eduardo Padilla Castillo[1], Priyansh Agarwal[1], Pulkit Kukreja[1], Russell Thomas[1], Boris Sartakov[1], Stefan Truppe[2], Gerard Meijer[1], and Sidney Wright[1] — [1]Fritz-Haber-Institute, Berlin, Germany — [2]Imperial College London, London, UK

Ultracold polar molecules have aroused great interest for their applications in testing fundamental physics and chemistry. Whilst there has been considerable success in associating ultracold diatomic molecules from laser-cooled atoms, these species are weakly bound and scarce in nature. A complementary approach is to laser cool molecules directly. So far, all diatomic and polyatomic species loaded into a magneto-optical trap (MOT) are spin-doublet molecules, and therefore chemically reactive. Moreover, their electronic structure only supports simple optical cycling from the first rotationally excited ($N = 1$) level.

Recently, we demonstrated the first MOT of a molecule with a (spin-singlet) $X^1\Sigma^+$ electronic ground state, aluminum monofluoride (AlF). We can routinely trap 6×10^4 AlF molecules via the deep ultraviolet $A^1\Pi \leftarrow X^1\Sigma^+$ transition, and, different to spin-doublet molecules, can straightforwardly select different rotational levels in the MOT. In this talk, I will provide a status update for the AlF MOT experiments, investigations of potential loss channels in the cooling cycle, and prospects for further cooling and trapping.

MO 8.5 Tue 12:15 P 105

Colder collisions for cleaner tomography of Feshbach resonances between atoms and molecules — •Karl P. Horn[1,2], Arijit Das[1], Yufeng Wang[1], Julia Narevicius[1,4], Meenu Upadhyay[3], Baruch Margulis[4], Daniel M. Reich[2], Markus Meuwly[3], Christiane P. Koch[2], and Edvardas Narevicius[1,4] — [1]Technische Universität Dortmund — [2]Freie Universität Berlin — [3]University of Basel — [4]Weizmann Institute of Science

Fundamental quantum effects are investigated at the interface between theory and experiment. Foremost amongst these are Feshbach resonances - observed, for instance, in collisions between rare gas atoms and a dihydrogen molecule ions (and their isotopomers). By launching collisions using Penning ionisation, coincidence measurement can yield a tomographic picture between incoming and outgoing quantum states [1]. Ab initio calculations convoluted to match the experimental resolution demonstrate good agreement with these experiments.

Until now, resolving contributions to the spectra due to individual initial partial waves and Feshbach resonances has been beyond experimental limitations [2]. The latest experiments demonstrate sufficient resolution to resolve these features and thereby test the validity of high-quality potential energy surfaces. By utilising Feshbach resonances characteristic to individual electronic structure methods and basis sets, a systematic comparison can be made between experiment and different levels of theory.

(1) Baruch Margulis et al. Science 380,77-81(2023).

(2) Karl P. Horn et al. JPCL 16 (31), 7862-7867 (2025).

MO 8.6 Tue 12:30 P 105

Electric-field control of atom-molecule Feshbach resonances — •Mara Meyer zum Alten Borgloh, Jule Heier, Fritz von Gierke, Baraa Shammout, Eberhard Tiemann, Leon Karpa, and Silke Ospelkaus — Leibniz University Hannover

We present our latest results on collisions between ^{23}Na^{39}K molecules and ^{39}K atoms, where we successfully observe Feshbach resonances between these scattering partners. For the first time in comparable systems, we demonstrate the ability to control the position of these resonances using electric fields. This allows us to investigate the electric field dependence of bound trimer states and assign specific quantum numbers to these states.

Our observations highlight a significant influence of the potassium atom on the molecule, despite the weak binding of the trimer state, which can be attributed to hindered rotation. These findings represent a new step in controlling atom-molecule interactions in ultracold gases and offer valuable insights into the behavior of molecular systems under external fields.

MO 8.7 Tue 12:45 P 105

Theory and experiments towards laser cooling of NH — •Daniel Roesch — TU Dortmund, Germany

Laser cooling of atoms is a well-established technique to reach very low temperatures and to generate degenerate quantum gases. Due to their more complex internal structure, molecules are much harder to laser cool. However, laser cooling of CaF, SrF, YO, YbF, BaF, AlF and SrOH has already been demonstrated and many other molecules are currently under investigation. We are working on laser cooling of ^{15}NH. This is a challenging molecule for laser cooling. While its light mass and cooling transition in the UV give rise to large momentum transfer for each absorbed photon, a long lifetime of the excited state and resulting narrow transition are posing considerable challenges. I will present results of hyperfine state resolved laser-induced fluorescence experiments on the cooling transition $A^3\Pi_0 \leftarrow X^3\Sigma^-$ for ^{15}NH as well as high resolution THz spectroscopy probing the $X^3\Sigma^-, N = 1 \leftarrow X^3\Sigma^-, N = 0$ rotational transition in the ground state. In addition to the experimental spectroscopy results I will also present results from laser cooling simulations using the pyLCP python package and machine learning optimization of laser cooling parameters.

MO 8.8 Tue 13:00 P 105

Towards a Dipolar BCS-BEC Crossover — •Eugen Dizer[1], Arthur Christianen[2], Xin Chen[1], and Richard Schmidt[1] — [1]Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institute for Theoretical Physics, ETH Zürich, Zürich, Switzerland

Dipolar Fermi gases are expected to show exotic phases of matter, such as the supersolid and the Wigner crystal phase. Their anisotropic long-range interactions make them also highly relevant for the study of unconventional superconductivity. In this work, we focus on the case of highly population-imbalanced dipolar Fermi gases to explore their few- and many-body physics. We analyze the quantum scattering of a single impurity in a dipolar Fermi sea, highlighting key differences from conventional short-range interaction models. Additionally, we discuss implications for the polaron-to-molecule transition and Anderson's orthogonality catastrophe, introducing a new theoretical framework to address this problem. Our results provide insights into the interplay between s- and p-wave pairing, and the emergence of supersolid phases, in the dipolar BCS-BEC crossover. We propose an experimental protocol to test the predictions in this work using ultracold molecules.

MO 9: Chirality II

Time: Tuesday 11:00–13:00 Location: P 110

Invited Talk MO 9.1 Tue 11:00 P 110

All-Optical Enantiomeric Conversion Observed in a Femtosecond Molecular Movie — •Nicolas Ladda, Fabian Westmeier, Tonio Rosen, Sudheendran Vasudevan, Simon Ranecky, Sagnik Das, Krishna Singh, Hendrike Braun, Jochen Mikosch, Thomas Baumert, and Arne Senftleben — Institute of Physics and CINSaT, University of Kassel, 34132 Kassel, Germany

We present the first observation of the enantiomeric conversion of an optically excited chiral molecule on the femtosecond timescale. Pumping the chiral molecule (methyl p-tolyl sulfoxide) into an electronically excited state with a deep-UV femtosecond laser pulse creates a vibrational wave packet, that can propagate to the other enantiomeric configuration due to a reduced inversion barrier [1]. By measuring time-resolved photoelectron circular dichroism (PECD), these molecular dynamics can be investigated in the gas phase, which provides an interaction-free environment. Advantageously, PECD, i.e., the forward/backward asymmetry of the photoelectron angular distribution with respect to the direction of propagation of ionizing circularly polarized light, is a strong (˜10%) effect and can be studied in an energy-resolved manner using a velocity map imaging spectrometer [2].

[1] W. Sun, I. Kleiner, A. Senftleben, M. Schnell, J. Chem. Phys. 2022, 156, 15, 154304.

[2] N. Böwering, T. Lischke, B. Schmidtke, N. Müller, T. Khalil, U. Heinzmann, Phys. Rev. Lett. 2001, 86, 1187

MO 9.2 Tue 11:30 P 110

Photoelectron Circular Dichroism in the Photodetachment of Deprotonated 1-Phenylethanol — •Viktoria Katharina Brandt, André Fielicke, Gerard Meijer, and Mallory Lee Green — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Photoelectron Circular Dichroism (PECD) is a chiroptical effect revealed in the angle-dependent photoemission of an electron from a chiral molecule, upon irradiation by circularly polarized light. PECD can provide insight into our understanding of electron dynamics, as this effect is acutely sensitive to the state of the molecule and the emission conditions of the electron. PECD within the photodetachment of anions has historically been understudied. Past studies of PECD in the photodetachment of anions have reported PECD effects averaged across multiple overlapping electron detachment channels represented by energetically similar tautomers, conformers, and electronic states. In such cases, the sensitivity of PECD to electron dynamics is a double-edged sword: PECD studies can only offer a wealth of information if one can disentangle the individual contributions to the overall measured PECD. Within this study, we measure the PECD effect in the photodetachment of a single electronic state of a single conformer of deprotonated 1-phenylethanol anion to explore the explicit effects of electron kinetic energy and vibrational state on the chiroptical effect within this photoemission regime.

MO 9.3 Tue 11:45 P 110

Robust Prediction of Plasmonic Enhanced Circular Dichroism — •Maria J. Weseloh[1], Mikael Kuisma[2], Tuomas Rossi[3], Xi Chen[4], and Patrick Rinke[1,5] — [1]Aalto University, Finland — [2]Technical University of Denmark, Denmark — [3]CSC - IT Center for Science, Finland — [4]Lanzhou University, China — [5]Technical University of Munich, Germany

Chirality can determine properties such as toxicity, making detection critical for health and environmental safety. Circular dichroism (CD) spectroscopy is a key technique for chiral discrimination but is often limited by weak chiral signals below measurable thresholds. Plasmonic enhancement of molecular circular dichroism by nanoparticles (peCD) enables detection of molecular chirality where conventional CD fails. Real-time time-dependent density functional theory (RT-TDDFT) in principle enables predictive peCD spectra, but in practice a fundamental issue arises: in the traditional length gauge, CD spectra depend on the arbitrary choice of coordinate-system origin - as highlighted in Phys. Rev. B 110, 115423 (2024). We overcome this limitation by implementing a velocity-gauge formulation of RT-TDDFT. Unlike the length gauge approach, where the dipole operator introduces explicit spatial dependence, the velocity gauge employs the momentum operator and removes this spatial dependence. Calculations across 27 distinct origins for molecules and nanoparticle-molecule systems demonstrate a robust origin insensitivity, even with moderately sized basis sets. Thanks to its computational efficiency, our method supports predictive and practical simulations of realistically large systems.

MO 9.4 Tue 12:00 P 110

Photoelectron circular dichroism modified by the Dynamic Stark effect — •Sudheendran Vasudevan[1], Anton N. Artemyev[1], Ignacio M. Casasús[2], Nicolas Ladda[1], Simon T. Ranecky[1], Sagnik Das[1], Tonio Rosen[1], Fabian Westmeier[1], Krishna Kant Singh[1], Daniel M. Haubenreisser[1], Eric Kutscher[1], Jochen Mikosch[1], Hendrike Braun[1], Luis Bañares[2], Philipp V. Demekhin[1], Arne Senftleben[1], and Thomas Baumert[1] — [1]Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany — [2]Dpto. de Química Física, Universidad Complutense de Madrid, Avenida de las Ciencias, 28040 Madrid, Spain

Photoelectron circular dichroism (PECD) is a highly sensitive, enantioselective probe of chirality that arises from electric-dipole interactions and appears as a forward/backward asymmetry in photoelectron angular distribution along the light propagation direction. In this work, we investigate how laser intensity affects the PECD of the chiral prototype molecule fenchone using bandwidth-limited near-UV pulses tuned between the 3s and 3p Rydberg states. Increasing intensity alters the Freeman resonances during the 2+1 REMPI process through dynamic Stark shifts and simultaneously reduces the observed PECD. Our time-dependent, single-center model suggests that the dynamic Stark effect mixes an increasingly large set of dipole-coupled virtual states into the effective polarizability of the intermediate state. This admixture of states with differing PECD signatures results in a partial cancellation and a net PECD approaching zero.

MO 9.5 Tue 12:15 P 110

In Situ Circular Dichroism Spectroscopy and Spatial Separation of Chiral Molecules — •Sejun An, Gerard Meijer, and Sandra Eibenberger-Arias — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Chirality is a fundamental symmetry property, yet enantiomers remain difficult to distinguish or control. Enantiomer-Specific State Transfer (ESST) provides a powerful route for enantioselective population control by driving a sequence of microwave transitions [1]. Recent advances in 2024 increased the ESST efficiency to 92%, enabling near-complete state-specific enantiomeric enrichment [2].

Here, ESST is extended toward in situ circular dichroism (CD) spectroscopy. Since the population of a quantum state can be enantioselectively controlled, CD measurements can be performed directly on a racemic mixture without switching laser polarization. This enables CD spectroscopy for chiral molecules that cannot be separated into pure enantiomers by conventional methods, and reduces systematic errors associated with polarization switching, thereby improving reproducibility and sensitivity.

Furthermore, ESST will be further advanced by rotational-state-selective ionization, enabling spatial separation of enantiomers. In this approach, the enantioselectively prepared rotational state is ionized, and the resulting ions can be separated by an external electric field.

[1] S. Eibenberger et al. Phys. Rev. Lett. 118, 123002 (2017)

[2] J. H. Lee et al. Nat. Commun. 15, 7441 (2024)

MO 9.6 Tue 12:30 P 110

Photoelectron Circular Dichroism of Aqueous-Phase Alanine — •Dominik Stemer and Bernd Winter — Fritz Haber Institute of the Max Plank Society, Berlin, Germany

Photoelectron circular dichroism (PECD) manifests as a forward-backward asymmetry in photoelectron flux upon photoionization of chiral molecules by circularly polarized light, and is an exquisitely sensitive probe of molecular chirality, capable of determining enantiomeric excess, but also of resolving differences in molecular conformation and charge state. Although the use of PECD to study chiral biomolecules under physiologically relevant conditions promises to shed light on otherwise difficult-to-access interactions, for example the nature of chirality transfer between a chiral solute and its first solvent shell, the application of PECD to liquid samples is practically challenging. We have previously demonstrated the possibility of measuring PECD for liquid microjets of the neat chiral liquid fenchone, and have more recently confirmed the applicability of PECD to aqueous solutions more generally. Here, we will report on our successful LJ-PECD experiments for core-level photoionization of aqueous-phase alanine, as well as on new results based on the chiral surfactant methylbenzylamine.

MO 9.7 Tue 12:45 P 110

Chiral Discrimination on Gate-Based Quantum Computers — •Sabre Kais[2] and Muhammad Arsalan Ali Akbar[1] — [1]Department of Electrical and Computer Engineering, and Department of Chemistry North Carolina State University, Raleigh, NC 27606 — [2]Department of Electrical and Computer Engineering, and Department of Chemistry North Carolina State University, Raleigh, NC 27606

We present a novel approach to chiral discrimination using gate-based quantum processors, addressing a key challenge in adapting conventional control techniques using modern quantum computing. Schemes such as stimulated rapid adiabatic passage (STIRAP) and shortcuts to adiabaticity (STAP) have shown strong potential for enantiomer discrimination; their reliance on analog and continuous-time control makes them incompatible with digital gate-based quantum computing architectures. Here, we adapt these protocols for quantum computers by discretizing their Gaussian-shaped pulses through Trotterization. We simulate the chiral molecule 1,2- propanediol and experimentally validate this gate-based implementation on IBM quantum hardware. Our results demonstrate that this approach is a viable foundation for advancing chiral discrimination protocols, preparing the way for quantum-level manipulation of molecular chirality on accessible quantum architectures

MO 10: Poster – Ultrafast Structural Dynamics

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 10.1 Tue 17:00 Philo 1. OG

Direct observation of uracil cation fragmentation via metastable intermediate — •Aditi Pradhan[1,2], Atilay Ayasli[1], Ivo S. Vinklárek[1], Hubertus Bromberger[1], Sebastian Trippel[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Chemistry, Universität Hamburg, Germany — [3]The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

Nucleobases are remarkably photostable biomolecules with complex relaxation dynamics at picosecond timescales [1], making them ideal test beds to explore ultrafast fragmentation dynamics with atomic-scale precision. We employ the versatile transportable endstation for controlled molecules (eCOMO) [2] to study isolated uracil molecules as well as hydrated clusters in a size-selected fashion [3]. Our photodissociation experiment in the strong-field regime reveals a metastable fragmentation pathway of uracil cation, enabled by 3D imaging beamplots. The findings are supported by lifetime estimates and accompanied by preliminary theoretical results.

[1]Nachtigallová *et int.* (4 authors), Lischka, *J. Phys. Chem. A*,**21** 115 (2011)

[2]Jin *et int.* (8 authors), Küpper, submitted (2024), arXiv:2406.16491 [physics]

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

MO 10.2 Tue 17:00 Philo 1. OG

Laser-Induced Electron Recollision in Molecular Targets Studied with a Reaction Microscope — •Martin Garro Gonzalez, Narayan Kundu, Julian Schröter, Janko Umbach, Horst Rottke, Arne Senftleben, and Jochen Mikosch — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Laser-driven electron recollision originates from strong-field ionization of atoms, molecules, and solids, where liberated electrons are accelerated by the oscillating laser field and driven back to the parent ion. This process underlies key strong-field phenomena, including non-sequential double ionization, high-harmonic generation, and laser-induced electron diffraction. A question of current interest is in which way electron recollision can be sensitive to the handedness of a chiral molecule. In recent proof of principle experiments, recollision-induced double ionization with elliptically polarized light has been shown to be chiral sensitive, and more recently photoelectron elliptical dichroism, arising from elastic rescattering, has demonstrated high chiral reponse. Here, we report advances in two recollision-driven phenomena. Using a reaction microscope, we investigate recollision-enhanced elliptical dichroism in chiral molecules with femtosecond strong-field studies of fragmentation and double ionization in methyl oxirane and limonene. Second, we will present our advances on controlling intensity- and wavelength-dependent Coulomb explosion of bromoiodomethane, investigating sequential and non-sequential channels.

MO 10.3 Tue 17:00 Philo 1. OG

Phase-dependent modulation of H2 dissociation in a bichromatic laser field — •Nikolas Rapp, Weiyu Zhang, Thomas Pfeifer, and Robert Moshammer — Max-Planck-Institut für Kernphysik, Heidelberg

The ionization and dissociation dynamics of H2 were investigated using a Reaction Microscope (ReMi). A femtosecond laser is shaped by a Spatial Light Modulator (SLM), enabling spectral control of the pulse in terms of amplitude, polarization, and phase. With the SLM, the laser pulse is split into two frequency components, with variable relative phase and temporal delay. The change of different dissociation pathways in terms of energy and yield with varying phase will be presented and compared to TDSE simulations.

MO 10.4 Tue 17:00 Philo 1. OG

Studying UV-induced dynamics in disulfide systems — •Sumukh Venkatesh Makam[1], James Merrick[2], Benoît Richard[3,4,5], Sergey Usenko[1], Robin Santra[3,4,5], Michael Meyer[1], Patrick A. Robertson[6], Matthew S. Robinson[1], and et al[1] — [1]European X-ray Free Electron Laser, Schenefeld, Germany — [2]Department of Chemistry, University of Oxford, Oxford, UK — [3]CFEL, DESY, Hamburg, Germany — [4]Department of Physics, University of Hamburg, Hamburg, Germany. — [5]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany. — [6]School of Chemistry, University of Nottingham, Nottingham, UK

Disulfide bonds (S-S) have a critical role in everyday chemistry, defining the tertiary structure of proteins. However, they undergo ultrafast fission when exposed to UV light leading to protein denaturation [1,2].

1,2-Dithiane is a model system that simulates the structural constraints of S-S bonds in proteins, and theoretical work predicts that it undergoes a cyclic ring-opening/closing process via S-S bond fission following UV (266 nm) excitation [2]. We present recent results obtained at the EuXFEL SQS Instrument in which these dynamics were captured via Coulomb Explosion Imaging.

In addition we also detail future plans to investigate the competing S-S and S-C fission processes following 200 nm absorption.

[1] A.B. Stephansen, et al., J. Am. Chem. Soc. 134, 20279 (2012).

[2] C.D. Rankine, et al., Phys. Chem. Chem. Phys. 18, 27170 (2016).

MO 10.5 Tue 17:00 Philo 1. OG

Formation of transient nanotips from plasmonically superheated silver nanocubes — •Nora Sigrist[1], Thomas Reichenbach[2], Alessandro Colombo[1], Bernd von Issendorf[3], and Daniela Rupp[1] for the SilverCubesAtSwissFEL-Collaboration — [1]ETH Zurich, Zurich, Switzerland — [2]IWM Fraunhofer, Freiburg, Germany — [3]University of Freiburg, Freiburg, Germany

The ultrafast structural dynamics of silver nanocubes are explored after excitation by an optical laser pulse tuned to their surface plasmon resonance. We used the intense X-ray pulses of SwissFEL to obtain single-shot single-particle coherent diffraction images (CDI) of their evolution. Under certain experimental conditions, we find the formation of complex transient geometries, six-legged nanostructures of about twice the size of the original nanocube. Matching this phenomenon with large-scale molecular dynamics simulations enables us to extract physical quantities of warm dense matter on the nanoscale, such as the viscosity of liquid silver at extreme temperatures and pressures, typically hardly accessible in a laboratory environment.

MO 11: Poster – Chirality

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 11.1 Tue 17:00 Philo 1. OG

Towards CD-Spectroscopy of Single Chlorosomes — •Stefan Goppelt[1], Lisa Günther[1], Thomas Jansen[2], Jasper Knoester[3], and Jürgen Köhler[1] — [1]Spectroscopy of soft Matter, University of Bayreuth, Germany — [2]University of Groningen, The Netherlands — [3]University of Leiden, The Netherlands

As one of the most efficient light-harvesting systems in nature chlorosomes (the light-harvesting aggregates of green-(non)-sulfur bacteria) are considered as a template for novel solar cells [1]. Among other techniques linear-polarization resolved fluorescence-excitation spectroscopy revealed molecular aggregates of cylindrical symmetry as the dominating secondary structural elements within the chlorosomes [2]. Development of circular-dichroism spectroscopy will allow to elucidate further structural details such as the diameter and the length of the cylindrical structures.

[1] S. Sengupta et al, Angew. Chem. Int. Ed., 51: 6378-6382 (2012)
[2] L. Günther et al, J. Phys. Chem. B, 122, 26, 6712*6723 (2018)

MO 11.2 Tue 17:00 Philo 1. OG

Towards the measurement of Photoelectron Circular Dichroism of (M)-[4] triangulane — •Tonio Rosen, Nicolas Ladda, Fabian Westmeier, Simon Ranecky, Sagnik Das, Sudheendran Vasudevan, Krishna Kant Singh, Hendrike Braun, Arne Senftleben, Jochen Mikosch, and Thomas Baumert — Universität Kassel

[n] Triangulanes are helically chiral molecules with structural helicity, providing a chiral scattering potential for electrons upon photoionization and a helical electron distribution in their highest occupied molecular orbital. Hence, these molecules are promising for investigating photoelectron circular dichroism (PECD) after resonance-enhanced multiphoton ionization in the gas phase. PECD is defined as a forward-backward asymmetry in photoelectron distribution with respect to the laser propagation direction in chiral molecules ionized with circularly polarized light. Using a velocity map imaging spectrometer, we aim to investigate the PECD of the smallest chiral triangulane, the [4] triangulane, in the 200- to 800 nm range. To this end, we want to employ gas chromatography, separating the enantiomers of a racemic mixture before their introduction into the experimental chamber. In this contribution, we will present the recent progress of this project.

MO 11.3 Tue 17:00 Philo 1. OG

Controlling the orientational degeneracy of rotational states in chiral molecules — •Elahe Abdiha, Shilpa Yadav, Sejun An, JuHyeon Lee, Boris G. Sartakov, Gerard Meijer, and Sandra Eibenberger-Arias — Fritz-Haber-Institut der Max-Planck-Gesellschaft; Berlin, 14195, Germany

We present recent experimental advances towards full enantiomer-specific control of the quantum states of chiral molecules using enantiomer-specific state transfer (ESST). Early studies on ESST reported only modest state-specific enantiomeric enrichment, limited to a few percent [1,2]. The main limitations are due to the thermal population of rotational states and their spatial degeneracy. Our group has overcome the limitation due to thermal population and achieved near-complete control of the enantiomers in a triad of rotational states containing the absolute ground state [3]. For this, we developed a new approach combining ultraviolet and microwave radiation to remove population from two out of three rotational states before applying ESST. In our recent work, we address the limitation due to spatial degeneracy when applying ESST to rotational states not including the absolute ground state. Here, M-state dependent Rabi frequencies impede the overall transfer efficiency when employing conventional pulse schemes. We incorporate theoretically tailored pulse schemes [4] and demonstrate enhanced control despite degeneracy. [1] Eibenberger et al. Phys. Rev. Lett. 118, 123002 (2017) [2] Pérez et al. Angew. Chem. Int. Ed. 56, 12512 (2017) [3] Lee et al. Nat. Commun. 15, 7441 (2024) [4] Leibscher et al. Commun. Phys. 5, 110 (2022).

MO 11.4 Tue 17:00 Philo 1. OG

Towards Circular Dichroism in Ion Yield and Electron Kinetic Energy on 3-Methylcyclopentanone — •Liliana M. Ramos Moreno[1], Deepak K. Pandey[1], Sagnik Das[1], Claus-Peter Schulz[2], Hendrike Braun-Knie[1], and Jochen Mikosch[1] — [1]Institut für Physik, Universität Kassel, Heinrich Plett Str. 40, 34132 Kassel, Germany — [2]Max Born Institute, Max-Born-Straße 2A, 12489 Berlin, Germany

The cyclic ketone 3-methyl cyclopentanone (3-MCP) is well-known for a strong Circular Dichroism in Ion Yield (CDIY) effect in resonance enhanced multiphoton ionization via the $\pi^* \leftarrow$ n transition. Coherent control of CDIY in 3-MCP using tailored femtosecond laser pulses has recently been demonstrated [1]. We now aim to build on this study to resolve the CDIY effect into different photoelectron kinetic energy bands. To this end we extend the twin focus approach [2], with two spatially separated foci of opposite and alternating circular polarization in an ion time-of-flight mass spectrometer, to Photoelectron Photoion Coincidence (PEPICO) spectroscopy [3]. Moreover, our temperature-variable molecular beam cluster source allows tuning the 3-MCP conformer composition within limits and, in the future, to explore effects oof micro-solvation via clustering individual water molecules to the chiral molecule.

[1] Das et al., Phys. Chem. Chem. Phys., 27, 8043-8051 (2025) [2] Ring et al., Rev. Sci. Instrum. 92, 033001 (2021) [3] Müller et al., JPCA 118, 8517 (2014)

MO 11.5 Tue 17:00 Philo 1. OG

Coherent Control of a chirality-modifying vibrational wave packet — •Nicolas Ladda, Fabian Westmeier, Tonio Rosen, Sudheendran Vasudevan, Simon Ranecky, Sagnik Das, Krishna Singh, Hendrike Braun, Jochen Mikosch, Thomas Baumert, and Arne Senftleben — Institute of Physics and CINSaT, University of Kassel, 34132 Kassel, Germany

Converting an enantiomer into the other configuration via an electronically excited state has recently been observed on the femtosecond timescale. Here, we want to present a coherent control scheme of the vibrational wave packet that is causing this transformation. A so-called pump-dump scheme is achieved by splitting the pump pulse into two parts and delaying one of them with a Mach-Zehnder interferometer. This allows for stopping the motion of the created wave packet by the pump pulse with the dump pulse at the desired delay. This results in the conversion of the enantiomer into its mirror configuration via the excited state [1] and subsequent fixation by deexcitation to the ground state. The process is studied by time-resolved photoelectron circular dichroism in the gas phase, providing an interaction-free environment and a large chiral observable [2].

[1] W. Sun, I. Kleiner, A. Senftleben, M. Schnell, J. Chem. Phys. 2022, 156, 15, 154304.

[2] N. Böwering, T. Lischke, B. Schmidtke, N. Müller, T. Khalil, U. Heinzmann, Phys. Rev. Lett. 2001, 86, 1187

MO 11.6 Tue 17:00 Philo 1. OG

Towards measuring the circular dichroism in the ion yield of selenofenchone via tailored femtosecond laser pulses — •Krishna Kant Singh, Sagnik Das, Nicolas Ladda, Sudheendran Vasudevan, Tonio Rosen, Fabian Westmeier, Arne Senftleben, Jochen Mikosch, Thomas Baumert, and Hendrike Braun — Institut für Physik, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Circular Dichroism (CD) is a powerful method for distinguishing enantiomers through their differential absorption of left- and right-circularly polarized light. This asymmetry can also manifest in their ionization yields, known as CD in ion yield (CDIY). We investigate this using our home-built Time-of-Flight mass spectrometer in a twin-peak measurement setup [1] to study how linear chirp influences the anisotropy [2]. The π^* * n transition in selenofenchone is red-shifted into the visible region (550*600 nm) and liquid-phase measurements indicate a pronounced CD effect. This makes the molecule particularly appealing for investigating CDIY, as technological controlling CDIY processes via tailored light fields is more readily achieved in the infrared or visible range. [1] T. Ring, et. al. Rev. Sci. Instrum., 2021, 92, 033001 [2] S. Das et. al., Phys. Chem. Chem. Phys., 2025, 27, 8043-8051

MO 11.7 Tue 17:00 Philo 1. OG

In Situ Circular Dichroism Spectroscopy and Spatial Separation of Chiral Molecules — •Sejun An, Gerard Meijer, and Sandra Eibenberger-Arias — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Chirality is a fundamental symmetry property, yet enantiomers remain difficult to distinguish or control. Enantiomer-Specific State Transfer (ESST) provides a powerful route for enantioselective population control by driving a sequence of microwave transitions [1]. Recent advances in 2024 increased the ESST efficiency to 92%, enabling near-complete state-specific enantiomeric enrichment [2].

Here, ESST is extended toward in situ circular dichroism (CD) spectroscopy. Since the population of a quantum state can be enantioselectively controlled, CD measurements can be performed directly on a racemic mixture without switching laser polarization. This enables CD spectroscopy for chiral molecules that cannot be separated into pure enantiomers by conventional methods, and reduces systematic errors associated with polarization switching, thereby improving reproducibility and sensitivity.

Furthermore, ESST will be further advanced by rotational-state-selective ionization, enabling spatial separation of enantiomers. In this approach, the enantioselectively prepared rotational state is ionized, and the resulting ions can be separated by an external electric field.

[1] S. Eibenberger et al. Phys. Rev. Lett. 118, 123002 (2017)

[2] J. H. Lee et al. Nat. Commun. 15, 7441 (2024)

MO 11.8 Tue 17:00 Philo 1. OG

Towards Photoelectron Circular Dichroism in the photodetachment from fenchone derived anions — •Viktoria Katharina Brandt, Kun Duan, André Fielicke, and Gerard Meijer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Photoelectron Circular Dichroism (PECD) is a chiral optical effect that manifests in the angle-dependent photoemission of an electron upon irradiation of a chiral molecule by circularly polarized light. The use of anions in PECD studies allows for pre-photodetachment mass selectivity and eliminates the need for X-ray based ionization sources or multiphoton ionization schemes. The use of anions also enables studies of PECD under conditions of photodetachment, a photoemission regime that has historically been understudied. Fenchone and its derivates have been extensively investigated using PECD, due to its rigid bicyclic structure, which limits the presence of additional isomers, as well as its non-toxicity and high availability. We present first steps in the study of PECD of fenchone derived anions. These anions are created in a plasma entrainment source where fenchone (FenH) reacts with hydride and hydroxide to form anions of three different masses, fenchone $-H^+$ (Fen^-), fenchone $+H^-$ ($FenHH^-$) as well as fenchone $+OH^-$ ($FenHOH^-$). The PECD and potential structures of these anions are presented.

MO 11.9 Tue 17:00 Philo 1. OG

A molecular source for probing ultrafast dynamics in chiral systems — •Akhila Jose[1], Juliette Leroux[1,2], Niclas Wieland[1], Sara Savio[1], Gunnar Petersen[1], Lasse Wülfing[4], Moritz Zander[1,3], Parth Patil[1,3], Filippa Dudda[1], Marius Thiem[1], Leonie Ashenbrenner[1], and Markus Ilchen[1,3] — [1]Department of Physics, Universität Hamburg, 22607 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, 22761 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Fakultät Physik, Technische Universität Dortmund, 44227 Dortmund, Germany

Chiral molecules are fundamental to life. They exhibit different interactions with other chiral systems, even though they share identical properties in achiral environment. Probing these differences requires measuring the photoelectrons and fragment ions produced after photo-dissociation. A double-sided velocity map imaging spectrometer enables simultaneous 4π detection of electrons and ions, providing correlated information on electron angular distributions and molecular fragmentation. To study intrinsic chiral behavior under realistic conditions, molecules must be examined in both isolated and liquid environments. This requires a molecular source that delivers high axial density for efficient ionization and high-quality imaging signals. Combining the newly developed molecular jet with a double-sided imaging spectrometer and tabletop laser or synchrotron radiation, we can resolve chiral effects, from photoelectron patterns to enantiomer-specific and phase-dependent behavior.

MO 12: Poster – Novel Experimental Approaches and Novel Theoretical and Computational Approaches

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 12.1 Tue 17:00 Philo 1. OG

Analysis of ultrafast structural dynamics based on single-shot XUV FEL data through deep learning — •Viktoria Chatrchyan[1], Alexander Magunia[2], Thomas Pfeifer[2], and Tiago Buckup[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls Universität Heidelberg, Germany — [2]Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Ultrafast time-resolved spectroscopy of core-electron excitation with extreme-ultraviolet (XUV) and x-ray free-electron lasers (FELs) is an effective approach to study structural dynamics and relaxation kinetics in atoms and molecules in real time. However, the kinetic analysis of such data is often accompanied by many challenges due to the complex, partially coherent nature of SASE FEL pulses. To compensate for the lack of control over exact machine parameters during a single experiment, the analysis is performed on averaged data from hundreds of single shot measurements described with statistical parameters. Thus, information about the direct impact of an individual laser pulse on a system is often lost. The goal of this work is to extract the exact correlation between single-shot laser pulse characteristics and the resulting changes in a molecular system. For this purpose, a deep neural network is being trained on transient absorption data and XUV FEL pulse spectra simulated using a partial-coherence method that predicts the structural dynamics of a system. This tool promises significant advantages for FEL science research allowing instantaneous and exact analysis of large amounts of data without omitting crucial information from single experiments.

MO 12.2 Tue 17:00 Philo 1. OG

Disentangling Nonlinear Signal Orders in Fluorescence-Detected Multidimensional Spectroscopy via Intensity Cycling — •Vishnu E. Krishnan, Stefan Mueller, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Ultrafast spectroscopic measurements inherently include contributions from higher-order terms of the perturbation series, which can obscure the interpretation of nonlinear signals. Recently, our group demonstrated that intensity-dependent measurements (intensity cycling) enable the recovery of clean nonlinear responses in transient absorption [1] and coherently detected multidimensional spectroscopy [2]. Herein, we extend this method to fluorescence-detected multidimensional spectroscopy, using CdSe-based nanoplatelets as model samples, and successfully extract clean nonlinear signals.

[1] P. Malý, J. Lüttig, P. A. Rose, A. Turkin, C. Lambert, J. J. Krich, T. Brixner, Nature 616, 280 (2023).

[2] J. J. Krich, L. Brenneis, P. A. Rose, K. Mayershofer, S. Büttner, J. Lüttig, P. Malý, T. Brixner, J. Phys. Chem. Lett. 16, 5897 (2025).

MO 13: Poster – Ultrafast Electronic Dynamics

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 13.1 Tue 17:00 Philo 1. OG

Time-resolved photoelectron spectroscopy of acetone using few-femtosecond pulses — Kate Robertson[1,2,3], Ammar B. Wahid[1], •Aurelien Sanchez[1,2,3], Sergey Riabchuk[1,2,3], Lorenzo Colaizzi[1], Erik Månsson[1], Terence Mullins[1,2,3], Vincent Wanie[1], and Francesca Calegari[1,2,3] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Germany — [3]Physics Department, Universität Hamburg

Few-femtosecond ultraviolet (UV) pulses are essential for tracking electron motion in electronically excited neutral molecules. Because UV light drives many key photochemical and biological reactions, the ability to generate pulses of such brevity opens a path to probing these processes with unprecedented temporal sensitivity. In this work, we report a time-resolved photoelectron spectroscopy study of acetone using 2.1-fs transform-limited UV pump pulses together with near-infrared probe pulses, yielding an overall temporal resolution of 5.6 fs. Acetone exhibits intricate Rydberg couplings that strongly shape its excited-state behavior. While earlier time-resolved measurements have examined these dynamics, their temporal resolution was insufficient to resolve processes evolving on a few- to tens-of-femtoseconds timescale. Our measurements uncover strong electronic and vibrational coherences and provide clear evidence for rapid relaxation into the $\pi\pi^*$ state. We observe a slow oscillation of 24 fs persisting for roughly 100 fs in the photoelectron signal, alongside a faster 3.2 fs modulation, which may reflect the presence of an electronic coherence.

MO 13.2 Tue 17:00 Philo 1. OG

ultrafast coherent dynamics in light-harvesting complexes from purple bacteria — •xinpeng xu[1], paul recknagel[1], alastair t. gardiner[2], richard j. cogdell[3], richard hildner[4], and jürgen köhler[1,5,6] — [1]Spectroscopy of Soft Matter, University of Bayreuth, Bayreuth 95440, Germany — [2]Institute of Microbiology of the Czech Academy of Sciences, Třeboň 379 01, Czech Republic — [3]School of Molecular Biosciences, Glasgow University, Glasgow G12 8QQ, U.K. — [4]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 3, Groningen 9747 AG, The Netherlands — [5]Bavarian Polymer Institute, University of Bayreuth, Bayreuth 95440, Germany — [6]Bayreuther Institut für Makromolekülforschung (BIMF), Bayreuth 95440, Germany

Photosynthetic purple bacteria accomodate peripheral light-harvesting complexes, typically termed LH2, for capturing solar energy. The species Rps. acidophila features two different antenna complexes, i.e. the B800-B850 LH2 when grown under high-light conditions (HL LH2) and the B800-B820 LH2 when grown under low-light conditions (LL LH2). The different spectral positions of the absorbing states of these complexes are tuned by the presence (HL LH2) or lack (LL LH2) of specific hydrogen bonds between the chromophores and the protein backbone. Here we investigate how the protein structure controls the excitonic energy levels and their ultrafast coherent dynamics.

MO 13.3 Tue 17:00 Philo 1. OG

Electronic relaxation dynamics of iron(III) complexes functionalized with chromophores — •Samira Dabelstein[1], Ansgar Döring[1], Miguel Andre Argüello Cordero[1], Lennart Schmitz[2], Jakob Steube[2], Matthias Bauer[2], Franziska Fennel[1], and Stefan Lochbrunner[1] — [1]University of Rostock, Rostock, Germany — [2]Paderborn University, Paderborn, Germany

Conventional photosensitizers for photocatalysis are usually made from rare and valuable precious metals. This has prompted the search for alternatives based on first-row transition metals. Iron-based photosensitizers are among these alternatives and emerge as potential candidates, but they are limited by their short-lived charge transfer states. One strategy to overcome this limitation is targeted ligand design. This study presents a series of emitting iron(III) complexes modified with chromophores, featuring either phenyl or anthracene groups, directly attached to the ligand backbone. The anthracene complex shows unexpectedly fast relaxation dynamics in solution, attributed to a charge transfer state extended over the entire ligand, which becomes accessible only after chromophore coplanarization [1]. To investigate this hypothesis further, the complexes were embedded in a polymer matrix to restrict conformational changes. Femtosecond transient absorption UV-Vis spectroscopy, revealed for both complexes decay dynamics differing from the solution case. The results support in the case of anthracene the hypothesis of an additional relaxation pathway driven by chromophore coplanarization.

[1] L. Schmitz et al., Inorg. Chem. 64 (2025), 14101.

MO 13.4 Tue 17:00 Philo 1. OG

Influence of Polymer Structure on Multi-Exciton Interactions in Different Squaraine Polymers — •Karina Heilmeier[1], Emely Freytag[2], Kateřina Charvátová[3], Federico Gallina[4], Stefan Mueller[1], Jacob J. Krich[4,5], Christoph Lambert[2], Pavel Malý[3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [4]Department of Physics, University of Ottawa, Ottawa, Ontario, Canada — [5]Nexus for Quantum Technologies, University of Ottawa, Ottawa, Ontario, Canada

Higher-order nonlinear signals in ultrafast spectroscopy provide unique information on the interactions of multiple excitons and their dynamics. Recently, we demonstrated how such signals can be extracted using intensity cycling in higher-order transient absorption (TA) measurements [1]. Here, we employ higher-order TA and fluorescence-detected two-dimensional spectroscopy to investigate multi-exciton interactions in two structurally different squaraine polymers built up of the same monomer but with different connectivity. This direct comparison allows us to reveal how the different polymer structures influence the exciton relaxation, transport and exciton–exciton annihilation dynamics.

[1] P. Malý, J. Lüttig, P. A. Rose, A. Turkin, C. Lambert, J. J. Krich, T. Brixner, Nature 616, 280 (2023).

MO 13.5 Tue 17:00 Philo 1. OG

Unraveling Strong Coupling and Excitonic Dipole Reorganization in Macrocyclic Squaraine Dimers via 2DES Anisotropy — •Yi Xu[1], Jonathan Herpich[2], Christoph Lambert[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland 97074 Würzburg

A macrocyclic squaraine (MSQ) consists of two covalently linked squaraine chromophores forming a torus-shaped π-conjugated ring that exhibits H-aggregate-like interactions. When two such macro-cycles associate to form an MSQ dimer, additional inter-macrocycle coupling arises, giving rise to new excitonic states with mixed H- and J-aggregate character, as revealed by UV-vis-NIR and CD spectra.

To probe how local squaraine transition dipole moments reorganize in the MSQ dimer, we employ polarization-resolved 2DES anisotropy. The anisotropy dynamics reveal a clear reorganization of transition dipole moments (TDMs), suggesting the emergence of delocalized excitonic dipoles spanning both macrocycles. Ongoing analysis aims to quantify the relative dipole orientation and the extent of electronic delocalization across the dimer.

These findings offer a microscopic view of dipole reorganization in hierarchical chromophore assemblies and demonstrate that 2DES anisotropy is a powerful tool for disentangling inter-macrocycle coupling and aggregate character in complex π-conjugated systems.

MO 13.6 Tue 17:00 Philo 1. OG

Circular dichroism yield measurements using a magnetic bottle electron spectrometer with twin-focus detection scheme — •Alexander Gerlach, Steffen Leinberger, Horst Rottke, Sagnik Das, Hendrike Braun, and Jochen Mikosch — Institut für Physik, Universität Kassel, Kassel, Germany

We employ time-of-flight (TOF) spectroscopy with a magnetic bottle to explore the circular dichroism (CD) of chiral molecules in the gas phase. Measuring the energy resolved electron yield for right- and left-circularly polarized light with femtosecond UV pulses allows to distinguish the excitation channels for enantiomeric molecular species.

For this purpose we use a modified twin-focus detection scheme [1], which separates the interaction regions of the two polarization states perpendicular to the TOF axis. An MCP delay-line detector is used to obtain the time and spatial distribution of the emitted photoelectrons from the investigated chiral molecule. First test measurements with this newly assembled electron spectrometer are presented, complementing the established CD ion yield measurements [1] for these systems.

[1] T. Ring et al., Rev. Sci. Instrum. 92, 033001 (2021)

MO 13.7 Tue 17:00 Philo 1. OG

Ultrafast Isomerization Dynamics of Amino-Azobenzene Molecules Probed by TRPES — •Alina Khodko[1,4], Artem Norenko[4], Matthew Mgbukwu[3], Evgenii Titov[2], Nataliia Kachalova[4], Valerii Voitsekhovych[4], Igor Dmytruk[4,5], Stefan Haacke[3], Oleg Kornilov[1], and Jérémie Léonard[3] — [1]Max Born Institute, Max-Born-Straße 2A, 12489 Berlin, Germany — [2]Institute of Chemistry, University of Potsdam, Germany — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, Strasbourg, France — [4]Institute of Physics NAS of Ukraine, Nauky Ave, 46, 03028, Kyiv, Ukraine — [5]Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska St., Ukraine, 01601, Kyiv, Ukraine

To access the isomerization dynamics of azobenzenes, Metanil Yellow molecules, time-resolved photoelectron spectroscopy (TRPES) were performed using 400 nm pump and 15th harmonic (23.5 eV) probe pulses. The experimental setup has been described [1]. The excited-state signal, integrated within the range from 2.4 eV to 5.2 eV, is modeled with a bi-exponential decay function. The fit yields the constants of around 0.5 ps and 5.2 ps. In general, the timescales from the TRPES experiments are in good agreement with the results derived from the transient-absorption spectroscopy (TAS). Based on DFT calculations, the dynamics are tentatively assigned to the S2 -> S1 conversion followed by relaxation to a long-lived state, the nature of which (possibly a TICT state) remains to be confirmed. This project was supported by Laserlab (PID: 26494). 1. E. Titov, et. Faraday Discuss., 2021.

MO 14: Members' Assembly

Time: Wednesday 13:30–14:00 Location: P 110

All members of the Molecular Physics Division are invited to participate.

MO 15: Interaction with strong or short laser pulses I (joint session A/MO)

Time: Wednesday 14:30–16:15 Location: N 2

Invited Talk MO 15.1 Wed 14:30 N 2

Cross-process interference in single-cycle electron emission from metal needle tips — •Anne Herzig[1], Peter Hommelhoff[2], Eleftherios Goulielmakis[1], Thomas Fennel[1], and Lennart Seiffert[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock, Germany — [2]Faculty of Physics, Ludwig Maximilian University Munich, 80799 Munich, and Department of Physics, Friedrich Alexander University Erlangen-Nuremberg, 91058 Erlangen, Germany

Photoelectron spectra from strong-field ionization exhibit energy cutoffs and interference patterns from direct and backscattered electrons. While cutoffs at 2 U_p and 10 U_p follow from the three-step model, observed fringe structures are usually linked to interference within either emission channel. However, cross-process interference (CPI) *between* direct and backscattered electrons remains largely unexplored. With single-cycle pulses limiting emission to one optical cycle [1] and nanotips directing electrons into a single half-space [2], conditions arise under which CPI can be clearly resolved.

In our recent study [3], we predict carrier-envelope-phase-dependent spectra with clear CPI signatures by comparing TDSE simulations with a trajectory model extended by quantum interference. The resulting fringe pattern encodes sub-cycle information on the near-field acceleration dynamics, highlighting CPI as a promising route toward ultrafast solid-state photoemission metrology.

[1] M.T. Hassan et al., Nature 530, 66-70 (2016)
[2] S. Zherebtsov et al., Nature Physics 7, 656-662 (2011)
[3] A. Herzig et al., https://arxiv.org/abs/2509.01524 (2025)

MO 15.2 Wed 15:00 N 2

Multiphoton ionization with three-dimensional laser fields — •Hans-Christian Ahlswede, Darius Köhnke, Tim Bayer, and Matthias Wollenhaupt — Carl von Ossietzky Universität Oldenburg

We report the first observation of free-electron angular momentum wave packets generated by atomic multiphoton ionization with bichromatic three-dimensional (3D) polarization-tailored ultrashort laser fields. These fields, created by the non-collinear superposition of two polarization-shaped pulses of different colors from a supercontinuum polarization pulse shaper, provide electric-field components along all spatial directions. The resulting photoelectron momentum distributions, recorded via velocity map imaging, demonstrate full 3D coherent control of electronic superposition states extending beyond the constraints of planar polarization fields by unlocking all dipole selection rules $\Delta m = 0, \pm 1$. As an application, 3D pump*probe fields are used to image previously unobserved photoelectron wave packets mapping spin-orbit dynamics of the potassium $3d$ fine structure doublet. Our shaper-based approach establishes a route to fully controllable 3D light fields for chiral-sensitive light-matter interactions and ultrafast spectroscopy.

MO 15.3 Wed 15:15 N 2

Towards a velocity-map-imaging spectrometer for ultracold atoms — •Lasse Paulsen[1], Julian Fiedler[1], Jette Heyer[1], Markus Drescher[1], Klaus Sengstock[1], Klaus Bartschat[2], Juliette Simonet[1], and Philipp Wessels-Staarmann[1] — [1]Center for Optical Quantum Technologies, Universität Hamburg, Hamburg, Germany — [2]Department of Physics and Astronomy, Drake University, Des Moines, USA

The intense electric field of femtosecond laser pulses enables the ultrafast creation of ions and electrons within an ultracold quantum gas. This opens new possibilities for investigating the dynamics of ionic impurities and atom-ion hybrid systems, provided that the kinematics of the ionization process are well understood.

Here we report on the characterization of an electron velocity-map-imaging spectrometer for ultracold quantum gases, as part of a novel coincidence detection unit including an ion microscope. For characterization a pulsed krypton gas jet is ionized by femtosecond laser pulses with a center wavelength of 511 nm and peak intensities around 6×10^{13} W/cm^2. The measured photoelectron momentum distribution is compared to theoretical predictions based on the solution of the time-dependent Schrödinger equation, which confirm the observed significant shifts in the photoelectron energies caused by the high peak intensities.

This work is funded by the Cluster of Excellence "CUI: Advanced Imaging of Matter" of the DFG - EXC 2056 - project ID 390715994 and by the NSF under project Nos. PHY-2110023 and PHY-2408484.

MO 15.4 Wed 15:30 N 2

Modeling ultrafast plasma formation in dielectrics — •Julia Apportin[1], Christian Peltz[1], Thomas Fennel[1], Misha Ivanov[2], and Anton Husako[2] — [1]Institute for Physics, Rostock, Germany — [2]Max Born Institute, Berlin, Germany

Laser induced damage in dielectrics due to short pulse excitation plays a major role in a variety of scientific and industrial applications, such as the preparation of 3D structured evanescently coupled wave-guides [1] or nano-gratings [2]. The corresponding irreversible material modifications predominantly originate from higher order nonlinearities like strong field ionization and plasma formation, which makes their consistent description imperative for any kind of theoretical modeling. In particular the associated feedback effects on the field propagation can have drastic implications.

We developed a numerical model, that combines a local description of the plasma dynamics in terms of corresponding rate equations for ionization, collisions and heating [3] with a fully electromagnetic field propagation via the Finite-Difference-Time-Domain method, adding self-consistent feedback effects like the sudden buildup of plasma mirrors. Considering laser pulses of constant energy (30 nJ), we investigate the influence of pulse duration and focus size on material modification and compare the resulting geometries, energy deposition and critical plasma volume.

[1] L. Englert et al, Opt. Express 15, 17855-17862 (2007)
[2] M. Alameer et al, Opt. Lett. 43, 5757-5760 (2018)
[3] B. Rethfeld, Phys. Rev. B 73 035101 (2006)

MO 15.5 Wed 15:45 N 2

Photoinduced transient symmetry breaking and non-linear anomalous Hall responses in centrosymmetric 2D materials — •Arkajyoti Maity, Ulf Saalmann, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, Dresden

We theoretically investigate the prospect of inducing a non-trivial, nonlinear Hall response in Dirac materials obeying both inversion and time-reversal symmetries, specifically pristine graphene. This is possible by creating a non-thermal electronic distribution in the system by driving it with a finite duration ultrafast sub-cycle laser pulse. The resultant non-equilibrium state, generated by non-adiabatic transitions induced by the laser, can be made to break the general trigonal (C3) symmetry of the Hamiltonian and hence allow for a second-order Hall response to a weak electric probe, closely related to the quantum geometry of the system

MO 15.6 Wed 16:00 N 2

High-harmonic generation in an organic molecular crystal — •Falk-Erik Wiechmann[1,2], Samuel Schöpa[1], Lina Marie Bielke[1], Svenja Rindelhardt[1], Serguei Patchkovskii[3], Felipe Morales[3], Maria Richter[3], Dieter Bauer[1,2], and Franziska Fennel[1,2] — [1]Intitute of physics, University of Rostock, 18059 Rostock, Germany — [2]Department of Life, Light and Matter, University of Rostock, 18059 Rostock — [3]Max Born Institute (MBI) for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

Recently, organic molecular crystals (OMCs) were introduced as a novel target class for high-harmonic generation (HHG)[1], bridging the gap between gas-phase and solid-state targets. In OMCs, neighboring molecules experience a weak van-der-Waals coupling, which leads to solid like features, e.g. a delocalization of the electronic states over several unit cells. The perfect inherent alignment of all molecules makes OMCs an ideal target class for high-harmonic spectroscopy of large organic molecules, as it avoids the need for extremely challenging alignment techniques that have so far prevented corresponding measurements in the gas phase. With a fundamental 4000 nm mid-IR beam reaching 0.99 TW/cm2 we demonstrate that HHG from Pentacene crystals is possible without imposing physical damage. Measurements of the harmonic yield as a function of the driving polarization direction reveal that the harmonic generation process is driven by intermolecular effects and not by the response of non-interacting aligned molecules.
[1] Wiechmann, FE. et al., Nat. Commun. 16, 9890 (2025)

MO 16: Poster – Attosecond Physics (joint session A/MO)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 16.1 Wed 17:00 Philo 1. OG

New 1D atomic model potential for more accurate high-order-harmonic-generation spectra — •Krisztina Sallai[1,2], Szabolcs Hack[1,2], Szilárd Majorosi[1], and Attila Czirják[1,2] — [1]The Extreme Light Infrastructure ERIC | ALPS Facility, Szeged, H-6728, Hungary — [2]University of Szeged, Szeged, H-6720, Hungary

Building on the favourable properties of previously used one-dimensional (1D) atomic model potentials, we introduced a new 1D Gaussian-windowed atomic model potential in [1] for simulating the quantum dynamics of a single active electron atom driven by a strong, linearly polarized near-infrared laser pulse. This new model potential upgraded the accuracy of 1D numerical simulations for single-atom high-order-harmonic-generation (HHG) spectra under commonly used driving laser pulse parameters. By combining two model potentials, we define the Gaussian windowed soft-core Coulomb (GSC) potential (with a =2.551 and b = 2) as

$V^{1D}_{GSC}(z) = V^{1D}_{SC}(z)\exp(-(z/a)^2) + V^{1D}_{MSC}(z)\left(1 - \exp(-(z/b)^2)\right)$.

The GSC potential offers an outstanding balance of accuracy and computational efficiency, enabling TDSE simulations that generate reliable HHG spectra within minutes in the $1.26 \times 10^{14} - 6.88 \times 10^{14}\,W/cm^2$ peak intensity range. Our research suggests that the GSC potential performs best when the Keldysh parameter is within $0.45 \leq \gamma \leq 1$ and the 1D ground state population loss simulated with the GSC potential, is not greater than 0.6 at the end of the laser pulse, which is well in line with most GHHG methods.

References: [1] K Sallai et al., Phys. Rev. A 110, 063117 (2024)

MO 16.2 Wed 17:00 Philo 1. OG

A rigorous and universal approach for highly-oscillatory integrals in attosecond science — •Anne Weber[1], Job Feldbrugge[2], and Emilio Pisanty[1] — [1]Attosecond Quantum Physics Laboratory, King's College London, WC2R2LS London, UK — [2]Higgs Centre for Theoretical Physics, University of Edinburgh, UK

Light-matter interactions within the strong-field regime, such as high-harmonic generation, typically give rise to highly-oscillatory integrals, which are often solved using saddle-point methods. Not only do these methods promise a much faster computation, but they also inform a more intuitive understanding of the process in terms of quantum orbits, as the saddle points correspond to interfering quantum trajectories (think Feynman's path integral formalism). Despite these advantages, a sound understanding of how to apply saddle-point methods to highly-oscillatory integrals in a rigorous way, and with algorithms which work uniformly for arbitrary configurations and laser drivers, remains lacking. This hinders our ability to keep up with state-of-the-art experimental setups which increasingly rely on tightly-controlled laser waveforms. Here, I will introduce the key ideas of Picard-Lefschetz theory – the foundation of all saddle-point methods – and their implementation. Using high-harmonic generation and above-threshold ionisation as examples, I will show how those ideas provide a robust framework for the fast computation of integrals, as well as a widely-applicable algorithm to derive the relevant semiclassical quantum orbits that underlie the physical processes.

MO 16.3 Wed 17:00 Philo 1. OG

Coulomb-corrected reconstruction of ionization and recombination times in high-order harmonic generation — •Mohammad Monfared and Manfred Lein — Institute for Theoretical Physics, Leibniz Universität Hannover, Hannover, Germany

Accurate attosecond-scale measurement of electron dynamics is fundamental to ultrafast science. The orthogonally polarized two-color (OTC) field technique enables the reconstruction of electron ionization and recombination times from high-order harmonic generation (HHG) spectra. However, established retrieval methods often neglect or utilize an oversimplified treatment of the Coulomb interaction, limiting their precision. In this work, we introduce a refined time-retrieval method that significantly improves the accuracy of reconstructing ionization and recombination times in OTC fields. We identify that one of the main time-retrieval equations, namely the condition used in earlier works to maximize the harmonic intensity as a function of the two-color delay, is only approximate and replace it with a more accurate stationarity equation. In addition, we incorporate Coulomb effects beyond the simple approximation of an instantaneous momentum kick by numerically integrating the Coulomb force and potential along the classical electron trajectories, providing a more physically consistent correction. We benchmark our method against exact time-dependent Schrödinger equation simulations and the analytical R-matrix theory. Our results demonstrate a substantial improvement in the accuracy of the retrieved ionization times, achieving near-perfect agreement with benchmark models especially for high-frequency probe fields.

MO 16.4 Wed 17:00 Philo 1. OG

Technical performance of the upgraded XUV and soft X-ray split-and-delay unit at FLASH1 — •Matthias Dreimann, Michael Wöstmann, and Helmut Zacharias — Center for Soft Nanoscience, Universität Münster

The split-and-delay unit at FLASH1, in operation since 2007, has been upgraded to meet the advances of increasing photon energies of FLASH1 since then. With the original design first experiments were performed in 2007 and the SDU was permanently incorporated in the BL2 at FLASH1 in 2010. The upgrade increases the spectral range of the SDU from former hv = 250 eV to now hv = 750 eV. Two different mirror coatings achieve a high transmission in the whole spectral range. The design is based on a three dimensional beam path and allows choosing the propagation via two sets of mirrors with different coatings. A carbon coating allows a total transmission on the order of T > 0.74 for photon energies between hv = 30 eV and hv = 200 eV at a grazing angle of 3.0° in the variable beam path. In the fixed beam path a shallower grazing angle of 2.5° is used, which yields a total transmission of T > 0.79. An Ni coating can be used to additionally cover a range up to hv = 750 eV. This results in a total transmission of typically T = 0.4 in the variable and T = 0.3 in the fixed beam path. The delay range of the new set-up is -1 ps < t < +9 ps with a subfemtosecond temporal delay.

MO 16.5 Wed 17:00 Philo 1. OG

Attosecond Streaking Spectroscopy: From Gas-Phase Dynamics to Adsorbed Molecules — •Ron Ducke, Sven-Joachim Paul, Maximilian Pollanka, Christian Schröder, Pascal Freisinger, Andreas Duensing, Reinhard Kienberger, and Maximilian Forster — Technische Universität München, Garching, Germany

We present the attosecond streaking setup established in our laboratory, designed to investigate time-resolved photoemission dynamics with high temporal precision. By using attosecond pulses, generated by HHG, we successfully determined absolute photoemission delays across a broad range of systems. In the gas phase, we review key results including absolute delays in the valence range of water and comparative studies of isosteric molecules, which elucidate the link between electronic structure and emission timing. Furthermore, a systematic analysis of iodoalkanes reveals the significant influence of the molecular environment on the emission from the iodine atom. Moving beyond the gas state, we discuss the photoemission delays of molecules adsorbed on crystal surfaces. Investigations of iodomethane and iodoethane on Pt(111) demonstrate how molecular orientation and surface interactions affect the measured delays compared to the gas phase. Finally, we present an outlook on our current measurements regarding e.g. Xenon and Neon.

MO 16.6 Wed 17:00 Philo 1. OG

Phase control in XUV-assisted high-order harmonic generation — •Zeinab Hardani and Manfred Lein — Leibniz University Hannover, Institute of Theoretical Physics,30167 Hannover, Germany

We investigate high-order harmonic generation (HHG) driven by a combined extreme-ultraviolet (XUV) pulse combined with a strong infrared (IR) laser field. Single-photon absorption of the XUV pulse releases the electron with well-defined initial conditions, while the IR field governs its motion in the continuum and its recombination with the parent ion. We evaluate the harmonic phase in XUV-assisted HHG and identify four main contributions: the strong-field phase, the Coulomb phase from the long-range potential, the recombination phase from the transition dipole, and an additional ionization phase associated with XUV-assisted emission. To quantify these contributions, we solve the one-dimensional time-dependent Schrödinger equation (TDSE) for an atomic model driven by combined IR+XUV fields and compare the extracted phase with the theoretical methods: strong-field approximation, analytical R-matrix, and scattering-theory predictions. In addition, we employ a classical model including the Coulomb potential and the XUV-imposed initial velocity to obtain ionization and recollision times, these recollision times agree with those inferred from the TDSE. Overall, we show that the XUV field shifts ionization and recombination to later times, thereby delaying harmonic emission and reshaping the phase of attosecond electron trajectories in agreement with both quantum simulations and classical modeling, and offering a flexible route to control XUV-triggered HHG in time.

MO 16.7 Wed 17:00 Philo 1. OG

Building a high-resolution XUV attosecond transient absorption spectrometer to observe time-dependent effects in atoms and molecules — •Noah L. Wach[1], Gergana D. Borisova[1,2], Christian Ott[1], and Thomas Pfeifer[1] — [1]Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — [2]Department of Physics, Lund University, P.O. Box 118, 22100 Lund, Sweden

Attosecond transient absorption spectroscopy (ATAS) has been extensively used to observe ultrafast electronic as well as vibrational dynamics in atoms and molecules[1,2]. Here, a combination of intense NIR femtosecond pulses, together with a high-harmonic-generated XUV pulse derived from them, is used to probe and control the systems quantum dynamics. We develop a new experimental setup, SHARP-XUV, which combines a conventional ATAS setup with a high-resolution XUV spectrometer in a Rowland configuration featuring a 3-meter arm length. This design is aimed to obtain an energy resolution of more than 10 000. Together with a time resolution of about a hundred attoseconds, we will be able to observe the complex dynamics where electronic or vibrational resonances lie extremely close and are hard to resolve with conventional XUV spectrometers. This setup will enable us to study the laser control of the overlapping series of highly doubly excited helium states as well as the laser-driven dynamics of increasingly closely spaced transitions near an ionization threshold.

[1] C. Ott et al., Nature 516, 374-378 (2014)

[2] G. Borisova et al., Phys. Rev. Research 6, 033326 (2024)

MO 17: Poster – Interaction with VUV and X-ray Light (joint session A/MO)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 17.1 Wed 17:00 Philo 1. OG

Temporal evolution of x-ray fluorescence of highly charged xenon ions under FEL irradiation — •Moritz J. Grunwald-Delitz[1], Thomas M. Baumann[1], Michael Meyer[1], Johan Söderström[2], and Jan-Erik Rubensson[2] — [1]European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden

We present the results of x-ray emission spectroscopy (XES) measurements on the interaction of intense x-ray free-electron laser pulses with xenon gas, aiming for a state-resolved exploration of non-linear multiphoton ionization and excitation processes. We utilize the 1D-imaging spectrometer [M. Agåker et al., J. Synchrotron Radiat., 31(5), 2024.] at the SQS instrument of European XFEL and its gas cell sample environment, which allows for studying Xe at a few mbar, a regime where, besides photon-driven processes, electron collisions start to contribute to the highly charged ion and excited state populations. Interestingly, this was not observed during prior studies on neon gas under similar conditions [S.-K. Son et al., Phys. Rev. A, 112(5), 2025, L051101.]. Our measurements monitor the evolution of these contributions over several nanoseconds after the XFEL pulse, revealing a distinct double-peak structure in the time-of-flight distribution.

MO 17.2 Wed 17:00 Philo 1. OG

Parametric Mössbauer Radiation Generated by the European XFEL Electron Beam — •Ze-an Peng, Christoph H. Keitel, and Jörg Evers — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

The ultranarrow nuclear resonances of Mössbauer isotopes enable precision spectroscopy and x-ray quantum optical applications, yet they make strong resonant excitation difficult with conventional x-ray sources. Parametric x-ray radiation (PXR), produced when relativistic electrons traverse a crystal, provides a high-quality, low-divergence x- ray source. When the crystal contains Mössbauer nuclei, spectrally narrow parametric Mössbauer radiation (PMR) can be generated under suitable conditions. We develop a general dynamical diffraction theory of PMR for arbitrary emission directions, covering both the conventional diffraction geometry and the more extreme grazing specular diffraction geometry. We show that the new geometry can substantially enhance PMR intensity due to specular diffraction of the electron virtual-photon fields at the crystal surface, which allows radiation to form predominantly outside the crystal and thus avoids strong absorption. We further apply the framework to superradiant PMR (SPMR) generated by microbunched XFEL electron beams, and introduce how superradiant amplification and geometric optimization combine to boost emission. The scheme applies broadly to PXR and PMR from both incoherent continuous- wave electron beam and the XFEL electron bunches, offering a pathway toward intense, coherent, and spectrally narrow Mössbauer x-ray sources.

MO 17.3 Wed 17:00 Philo 1. OG

Microcrystalline and thin layers for precision spectroscopy — •Simon B. Diewald[1], Jonas Stricker[1,2], Dennis Renisch[1,2], and Christoph E. Düllmann[1,2,3] — [1]JGU Mainz, Deutschland — [2]HI Mainz, Deutschland — [3]GSI Darmstadt, Deutschland

^{232}ThF$_4$ is a promising host material for high-precision spectroscopy experiments related to the realization of a solid-state nuclear clock based on the $^{229\mathrm{m}}$Th isomer. We present a compact method for producing thin and microcrystalline ^{232}ThF$_4$ layers on silicon, CaF$_2$, MgF$_2$, and stainless-steel substrates via thermal evaporation in an ohmic furnace. The produced layers were characterized regarding their homogeneity and provide samples suitable for future high-precision vacuum-ultraviolet spectroscopy. The method provides homogeneous samples suitable for various high-precision spectroscopy and nuclear-physics applications.

MO 17.4 Wed 17:00 Philo 1. OG

Accessing ultrafast electron dynamics with single-shot single-particle diffraction imaging and spectroscopy — •Indrani Dey, Jasper Boultwood, José gómez Torres, Frederic Ussling, Yves Acremann, Isabelle Bolliers, Ehsan Hassanpour Yesagi, Linos Hecht, Katharina Kolatzki, Mario Sauppe, Simon Wächter, Changji Pan, Jannis Lehmann, Alessandro Colombo, Björn Senfftleben, and Daniela Rupp — Nanostructures and Ultrafast X-Ray Science, ETH Zurich

Ultrafast electron dynamics are in principle imprinted in diffraction patterns of single nanoparticles but they are difficult to extract. We have developed high-harmonic generation based single-shot single-particle diffractive imaging in the lab with excellent temporal stability and resolution. To gain access to ultrafast laser-driven changes in the electronic properties of an isolated nanoparticle, also the spectral distribution of the diffracted light needs to be recorded, as it reflects the static and dynamic interaction of the intense XUV pulse with the target. It is also crucial for accurate phase retrieval and structural reconstruction, as multi-harmonic contributions blur fine details. We discuss the design and setup for simultaneous recording of single-shot diffraction patterns and spectrum of free-flying particles and present first results. The development of Coherent Diffraction Imaging and Spectroscopy has the potential to enable also novel XFEL-based experiments with few- and sub-femtosecond pulses.

MO 18: Poster – Interaction with Strong or Short Laser Pulses (joint session A/MO)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 18.1 Wed 17:00 Philo 1. OG

Bound-free electron-positron pair production in combined Coulomb and constant crossed electromagnetic fields — •Svea Remme, Alexandra Eckey, Selym Villalba-Chavez, Alexander B. Voitkiv, and Carsten Müller — Institut für Theoretische Physik I, Heinrich-Heine-Universität Düsseldorf

Bound-free electron-positron pair production by a highly charged bare ion in the presence of a strong constant crossed electromagnetic field is studied. We apply two different methods to calculate the pair production rate: (i) a quasiclassical tunneling theory and (ii) a strong-field approximation, both equipped with appropriate Coulomb correction factors. The resulting rate is shown to depend nonperturbatively on both the Coulomb field of the ion and the constant crossed field.

MO 18.2 Wed 17:00 Philo 1. OG

Time-delay in Tunnel-Ionization and barrier-suppression ionization — •Ossama Kullie — Theoretical Physics, Institute for

Physics, Department of Mathematics and Natural Science, University of Kassel, Germany.

In previous work, we presented tunnel-ionization model [1,2], in which we showed a real tunneling time-delay picture that agrees well with the experimental results in the adiabatic [1] and nonadiabatic [3] field calibrations. In addition, we showed that the tunnel-ionization time exhibits a universal behavior consistent with Winful's unified tunneling picture [4], which amounts to determine the barrier time-delay with good agreement with the experimental result and it corresponds to the interaction time [5]. Barrier-suppression ionization is a phenomenon in strong-field physics where a high-intensity laser field completely flattens the potential barrier, allowing an electron to escape an atom or molecule without the need for quantum tunneling. In the present work, based on our model [1] and the findings of recent work [5], we extend our time-delay model to include the regime of barrier-suppression ionization. [1] O. Kullie, Phy. Rev. A 92, 052118 (2015). [2] O. Kullie, Annals of Physics 389, 333 (2018). [3] O. Kullie and I. A. Ivanov, Annals of Physics 464, 169648 (2024). [4] H. Winful, Phys. Rev. Lett. **90**. 023901 (2003). [5] O. Kullie, J. Phyis. Commun. 9, 015003, (2025).

MO 18.3 Wed 17:00 Philo 1. OG

Investigation of Interactions at relativistic laser intensities with Highly Charged Ions — •Stefan Ringleb[1], Manuel Vogel[2], Sugam Kumar[3], Stefan Kiesel[4], and Thomas Stöhlker[1,2,4] — [1]Friedrich-Schiller Universität Jena — [2]GSI Helmholtzzentrum für Schwerionenforschung Darmstadt — [3]Inter-University Accelerator Centre, New Delhi, India — [4]Helmholtzinstitut Jena

Interaction of high-intensity lasers with highly charged ions is a widely explored field theoretically. In contrast, there is still a lack of experimental data on the interaction with highly charged ions, with most experiments to date focusing on high-intensity laser ionization of initially neutral gases. In our working HILITE setup, highly charged ions prepared for ion targets in a defined initial quantum state containing between 5,000 and 25,000 ions. We have elaborated techniques for ion-cloud preparation regarding fast ion cooling in axial direction and ion number. We have investigated the radial self arrangement of the ions to maximise the ion number in the laser volume. Currently, an experiment at the 200 TW femtosecond Laser system JETi200 is in operation to investigate the ionization dynamics at relativistic laser intensities. In the experiment, we will focus on hydrogen-like ions which can be described precisely by theory. This will also allow for the intensity determination in the laser focus, as this is the less accurate determined parameter in laser experiments. The setup is designed to enable experiments of laser-ion interaction with high accuracy and allow the test of laser-ionisation models for many-electron systems.

MO 19: Poster – Contributions to SYLC

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 19.1 Wed 17:00 Philo 1. OG

Femtosecond transient circular dichroism spectroscopy and transient circularly polarized luminescence of chiral copolymer thin films — •Kawon Oum and Thomas Lenzer — University of Siegen, Physical Chemistry 2, Adolf-Reichwein-Str. 2, 57076 Siegen

We have recently developed an experimental methodology enabling the simultaneous recording of transient absorption (TA) and transient circular dichroism (TrCD) responses of photoexcited systems across the ultraviolet-visible spectral range (260-700 nm) with a time resolution of ca. 100 fs. This approach has been applied to chiral polyfluorene copolymer thin films exhibiting intrinsic [1] and induced supramolecular chirality,[2,3] where exceptionally strong circular dichroism signals of up to 16000 mdeg and dissymmetry factors approaching 0.7 were observed. Complementary steady-state and transient circularly polarized luminescence (TrCPL) studies reveal a remarkable sign inversion of both CD and CPL signals with increasing film thickness and annealing temperature, attributed to structural reorganization within the chiral supramolecular phase.[4] The pronounced chiroptical activity of these films highlights their potential for optoelectronic applications, particularly in OLEDs with intrinsic circularly polarized emission.

[1] M. Morgenroth et al., Nat. Commun. 2022, 13, 210. [2] M. Morgenroth et al., Angew. Chem. Int. Ed. 2022, 61, e202203075. [3] D. Gust et al., Sci. Rep. 2024, 14, 12694. [4] D. Gust et al., ChemPhotoChem 2025, e202500196.

MO 19.2 Wed 17:00 Philo 1. OG

Ultrafast TACOS — •Justas Terentjevas[1,2], Patricia Vindel-Zandbergen[3], Laura Rego[2,4,5], Felipe Morales[1], Andrés Ordóñez[2], Olga Smirnova[1,6], and David Ayuso[1,2] — [1]Max-Born-Institut, 12489 Berlin, Germany — [2]Department of Physics, Imperial College London, SW7 2BW London, UK — [3]Department of Chemistry, New York University, New York 10003, New York, USA — [4]Instituto Madrileno de Estudios Avanzados en Nanociencia (IMDEA Nano), Cantoblanco 28049, Madrid, Spain — [5]Departamento de Quimica, Universidad Autonoma de Madrid, 28049 Madrid, Spain — [6]Technische Universitat Berlin, 10623 Berlin, Germany

We introduce TACOS - Terahertz-Assisted Chiro-Optical Spectroscopy - a novel approach for ultrafast chiral recognition. We show that a terahertz field can electronically orient a medium of randomly oriented chiral molecules to twist the nonlinear response to an ultrashort optical pulse in a highly enantiosensitive manner. This process leads to the emission of elliptically polarised light at new optical frequencies that records the molecular handedness via purely electric-dipole interactions. The long wavelength and period of the terahertz pulse enable spatial coherence across the interaction region and a substantial degree of electronic orientation during the interaction of the molecules with the ultrashort optical pulse. TACOS does not require optical carrier-envelope phase stability or vacuum conditions, thus opening new avenues for ultrafast and highly efficient chiral sensing and manipulation.

MO 19.3 Wed 17:00 Philo 1. OG

Detection and control of molecular chirality in molecular ensembles — •Alexander Blech[1], Loren Greenman[2], Reinhard Dörner[3], and Christiane P. Koch[1] — [1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [2]Department of Physics, Kansas State University, Manhattan, KS, USA — [3]Institut für Kernphysik, Goethe-Universität, Frankfurt am Main, Germany

Photoelectron circular dichroism (PECD) - the forward-backward asymmetry in the photoelectron angular distributions of chiral molecules upon ionization with circularly polarized light - can detect molecular chirality in randomly oriented molecules with high sensitivity. With orientation, also achiral molecules yield PECD. This raises the question whether and if so, under which conditions, PECD signals unequivocally molecular chirality. We address this question through symmetry analysis and show that, when combined with rotational excitation using three mutually orthogonal polarization directions, PECD can reveal chirality even in racemic mixtures. Whereas such sequences of static and non-resonant fields yield PECD also for certain achiral molecules, microwave three-wave-mixing cycles can, in principle, unambiguously detect chirality in arbitrary molecular ensembles. Finally, we demonstrate that fields with three orthogonal polarization directions can not only detect but also induce chirality via chiral rotational dynamics, offering a new pathway for laser-based control of molecular handedness.

MO 20: Poster – Molecular Collisions and Kinetics

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 20.1 Wed 17:00 Philo 1. OG

MOCCA: A molecule camera for the position and energy resolved detection of neutral molecule fragments — •N. Fiedler[1], A. Fleischmann[1], C. A. Jakob[2], D. Kreuzberger[1], A. Özkara[1], D. Hengstler[1], A. Reifenberger[1], L. Gastaldo[1], P. Martini[3], S. Rosén[3], H. Zettergren[3], O. Novotný[2], H. T. Schmidt[3], and C. Enss[1] — [1]Kirchhoff Institute for Physics, Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg — [3]Department of Physics, Stockholm University

The MOCCA detector is a high-resolution camera for neutral molecule fragments with kinetic energies in the keV range. It features several thousand pixels based on metallic magnetic calorimeters and is read out using SQUIDs. To reconstruct the kinematics of electron-ion and ion-ion reactions, MOCCA measures both the energy and the impact position of molecular fragments incident on the detector, even with multiple particles hitting the detector simultaneously. The latest fabricated version is currently being deployed at the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, where molecular ions are stored and prepared in their rotational and vibrational ground states, allowing detailed studies of electron-ion interactions. We present plans for integrating the 11.5k-pixel MOCCA-Quattro detector system into the Double ElectroStatic Ion Ring ExpEriment (DESIREE) at Stockholm University, which enables mutual neutralization of ions at extremely small relative velocities. This will significantly enhance studies of neutralization processes in complex molecules prepared in their quantum ground state.

MO 20.2 Wed 17:00 Philo 1. OG

Insights into the activation of small molecules by transition metal ions — Marcel Meta, Maximilian Huber, •Maurice Birk, Martin Wedele, Boris Heeb, and Jennifer Meyer — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

A model process for single atom catalysis can be the study of isolated transition metal ion molecule reactions in the gas phase [1,2]. Here, we present studies of the dynamics on the activation of small organic molecules by transition metal cations. Nominally spin-forbidden reactions proceed via intersystem crossing (ISC) in the presence of such metal cations. The impact of ISC on the dynamics is studied by collaborative effort combining experiment and theory.

We used crossed-beam velocity map imaging to measure differential cross sections for the activation of methane and carbon dioxide with different transition metal cations [3,4]. These reactions show dominantly indirect dynamics which is associated to the formation of a long-lived intermediate complex. In addition recent theoretical studies confirmed our observations regarding the reaction with Ta^+ and methane which revealed that the bottleneck of this reaction is ISC between the quintet and triplet states.

[1] D. K. Böhme, H. Schwarz, Angew. Chem. Int. Ed. 2005, 44, 2336; [2] H. Schwarz, Catal. Sci. Tech. 2017, 7, 4302; [3] M. Meta, Faraday Discuss. 2024, 251, 587; [4] M. Meta et al., J. Phys. Chem. Lett. 2023, 14, 24, 5524

MO 20.3 Wed 17:00 Philo 1. OG

Low-energy dynamics of the H_2^+(v = 2) + Ar reaction probed by velocity map imaging — •Jerin Judy, James K. Bateman, Dasarath Swaraj, Fabio Zappa, Viviane C. Schmidt, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Crossed-beam experiments combined with the velocity map imaging (VMI) technique are a robust tool for obtaining energy- and angle-resolved differential cross sections [1]. Here, we report low-collision-energy studies on the reaction between H_2^+(v = 2) and Ar. The reactant ion, H_2^+, is produced predominantly in its second excited vibrational state using a (3+1) REMPI scheme. The reaction proceeds through two pathways-charge transfer and proton transfer-which we probe via Ar^+ and ArH^+, respectively. The charge transfer pathway exhibits a quasi-energy resonance between reactants and products. The velocity map images, together with the extracted product internal-energy and angular distributions, provide new detailed insights into the underlying reaction mechanisms.

[1] R. Wester, Phys. Chem. Chem. Phys. 16, 396 (2014).

MO 20.4 Wed 17:00 Philo 1. OG

Three-body reactions in cryogenic multipole traps — •Miriam Westermeier, •Gregor Rack, Michael Hauck, Sruthi Purushu Melath, Samuel J. M. White, Christian Sprenger, Robert Wild, Eric Endres, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Three-body (3B) reactions are relevant for many different topics, such as atmospheric physics and cluster physics, especially at higher gas densities. As benchmarks for theoretical calculations, the 3B reaction of Ar^+ + Ar + Ar and of alkali-water complexes are studied. The versatility of cryogenic ion traps makes them suitable for studying these 3B reactions and their temperature dependence [1, 2]. In our group, 3B reactions are researched on two different setups, both containing a cryogenic multipole trap. One setup is equipped with an electrospray ionization (ESI) source and the other with a plasma source. ESI sources are efficient in the production of water clusters, allowing the study of 3B reactions of these cluster ions. The ESI setup is currently undergoing changes to make it suitable for the higher pressures needed for the 3B reactions. The plasma source allows for the ionization of atoms with high ionization energy, and the trap has been optimized to study reactions with very low reactions rates. The 3B reaction Ar^+ + Ar + Ar is studied on this setup and the recorded data shall be presented, together with an overview of the current experiments.

[1] S. Schlemmer *et al.*, J. Chem. Phys. **116**,11 (2002)

[2] R. Wild *et al.*, J. Phys. Chem. A **125**,39 (2021)

MO 21: Poster – Cluster and Nanoparticles (joint session MO/A)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 21.1 Wed 17:00 Philo 1. OG

Penning ionization and direct photoionization of Mg and Na doped in helium nanodroplets — •Rajni Rajni[1], Narcis-Silviu Blaj[1], Asbjorn Ornemark Lagdsmand[1], Marcel Mudrich[1], Ltaief L. Ben[2], Niklas Scheel[2], and Henrik Pedersen[2] — [1]Institute of Physics, University of Kassel, D-34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

We investigate the direct photoionization and Penning ionization of alkali (Na) and alkaline-earth metals (Mg) embedded in superfluid helium nanodroplets under irradiation with extreme ultraviolet (XUV) synchrotron radiation that resonantly excites the He droplets. Helium is a well-suited system for studying indirect ionization processes due to the simple electronic structure of He, well-resolved electron spectra, weak interaction with embedded species, efficient pick up of molecules and controlled aggregation inside the nanodroplets. We measured spectra of all electrons and of electrons recorded in coincidence with specific ions for He nanodroplets doped with Mg and Na atoms. For Na, the Penning ionization electron spectrum is well resolved but shifted due to attractive interaction of the Na atom and the excited He* (short-range interatomic Coulombic decay). For Mg, we observe a pronounced enhancement of shake-up ionization where an excited Mg^+ ion is produced in the Penning process. Shake-up states are only weakly present in direct photoelectron spectra.

MO 21.2 Wed 17:00 Philo 1. OG

Tracking Microhydration of Salt Molecules in Helium Nanodroplets and Commissioning a New Nanoparticle Injector System — •Mikkel Mortensen[1], Niklas Scheel[2], Marcel Mudrich[2], Henrik B. Pedersen[2], and Ltaief B. Ltaief[2] — [1]Institute of Physics, Kassel University — [2]Department of Physics and Astronomy, Aarhus University

The solvation of NaCl molecules in water, is an important process in chemistry. However, microscopic structures and energetics of the hydration complexes remain to be investigated. A recent study has quantified the number of water molecules needed, to form a complete hydration shell around NaCl in helium nanodroplets using Penning Ionization Electron Spectroscopy (PIES)[1]. Building upon this study, we investigate the microhydration dynamics of KBr, NaBr, and NaCl under comparable conditions at the XUV synchrotron light source, ASTRID 2. Our PIES measurements aim to investigate how different ionic constituents affect hydration structure and stability.

Furthermore, we are commissioning a new nanoparticle injector based on an aerodynamic lens system for producing aerosol beams of salt nanoparticles. This development will allow us to do experiments on salt hydration and electron spectroscopy in aerosols, including interactions with XUV radiation at ASTRID.

[1] L. B. Ltaief et al., submitted (2025), arXiv.2510.22000

MO 21.3 Wed 17:00 Philo 1. OG

XUV photoionization of Microhydrated Biomolecules — •Niklas Scheel[1], Ltaief Ben Ltaief[1], Henrik B. Pedersen[1], and Marcel C. Mudrich[2] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute of Physics, University of Kassel, 34132 Kassel, Germany

Microhydrated biomolecules serve as valuable model systems for studying radiophysical processes in biologically relevant complexes, offering insights into the mechanisms of radiation damage in biological tissue. In this work, we present photoelectron-photoion coincidence (PEPICO) spectra of XUV-irradiated microhydrated thymine and uracil clusters, measured using the electron ion double-imaging endstation XENIA[1] at the ASTRID2 synchrotron.

We investigate outer-valence photoionization, confirming that attached water molecules stabilize the DNA bases against fragmentation[2] by acting as an efficient heat bath. At the same time, the data reveal a charge-transfer mechanism from the DNA base to the water: a charge hole initially created on a water moiety ultimately localizes on the DNA base.

Finally, we will present PEPICO spectra recorded at higher photon energies. These measurements probe inner-valence photoionization, where double ionization becomes accessible, leading to pronounced fragmentation and involving Intermolecular Coulombic Decay (ICD) as an efficient relaxation pathway.

[1] B. Bastian et al., Rev. Sci. Instrum., 2022, 93, 075110

[2] J. D. Asmussen et al., PCCP, 2023, 25, 24819-24828

MO 21.4 Wed 17:00 Philo 1. OG

Novel Apparatus for Synchrotron X-ray Photoelectron Spectroscopy of Size-Selected Gas-Phase Clusters — Lotar Kurti, Phillip Stöcks, Fabian Bär, Lukas Weise, and •Bernd v. Issendorff — Physikalisches Institut, Universität Freiburg, Freiburg, Germany

A newly developed apparatus enables X-ray photoelectron spectroscopy on mass-selected cluster ions at synchrotrons. The heart of this system is a liquid nitrogen-cooled linear Paul trap, where stored cluster ions interact with synchrotron radiation. The emitted electrons are guided by a specially designed magnetic field into a Hemispherical Energy Analyzer, where the photoelectron spectra are recorded. Clusters are produced in a magnetron cluster source, mass-selected using a quadrupole mass spectrometer, and then introduced into the linear ion trap. This setup will allow for element-specific binding energy measurements of core levels and hence detailed insights into the chemical bonding of pure and mixed metal and semiconductor clusters. In this contribution, we present the current status of the new apparatus and some initial commissioning results.

MO 21.5 Wed 17:00 Philo 1. OG

Single-shot imaging and modeling of individual water nanodroplets with an intense extreme ultraviolet laboratory source — •Lea Schüpke[1], José Gómez Torres[1], Linos Hecht[1], Frederic Ussling[1], Alessandro Colombo[1], Katharina Kolatzki[1], Indrani Dey[1], Changji Pan[1], Isabelle Bollier[1], Constantin Koch[1], Ehsan Hassanpour[1], Yves Acremann[1], Mario Sauppe[1], Björn Senfftleben[1], Hanchao Tang[2], Arnab Choudhury[2], Bruce Yoder[2], Ruth Signorell[2], and Daniela Rupp[1] — [1]ETH Zürich, DPHYS — [2]ETH Zürich, DCHAB

Our unique high-intensity extreme ultraviolet (XUV) beamline enables flash-imaging of individual free-flying nanoparticles in a lab environment, thus avoiding the severe access limitations of large-scale facilities. We have started to investigate the freezing dynamics of supercooled water droplets between few 100 nm and few μm in diameter. This size range is mostly unexplored due to the lack of suitable imaging methods. In this work, Mie-simulations are discussed that allow to understand subtle changes in the diffracted light distribution caused by aggregate state changes and droplet sizes.

MO 21.6 Wed 17:00 Philo 1. OG

Detailed investigation of unexpected photoelectron spectra via angle-resolved spectroscopy of noble metal clusters — •Steve Takouan Tchounga, Lukas Weise, and Bernd von Issendorff — Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany

Angle-resolved spectroscopy provides an important test of the theoretical description of clusters since these spectra carry more information than the bare electron binding energies. Specifically, the anisotropy of photoelectron spectra depends on the angular momentum state [1, 2].

The presented analysis utilizes the additional information from angle-resolved spectroscopy to gain a better understanding of the electronic structure of the cluster. For Au_{33}^- an electronic shell closing is expected, leading to the opening of a new shell for Au_{34}^-. The angular momentum character of this new shell is not in accordance with a simple shell model.

The Issendorff's model [2] was utilized to gain insight into the character of the orbital involved in the premature shell closing of Cu_{91}^-. The β parameter curve for this orbital exhibits a clear f-type character, indicating a premature filling of the next shell. The reason for this premature shell closing cannot be identified by this result, but the additional information on the character should help in finding the reason.

[1] Bartels et al., Science, 323, 5919 (2009). [2] Piechaczek et al., Phys. Rev. Lett. 126, 233201 (2021). [3] Bartels et al., Phys. Rev. A 88, 043202 (2013).

MO 21.7 Wed 17:00 Philo 1. OG

HHG Coherent Diffraction Imaging of water nanodroplets — •José Gómez Torres[1], David Biner[1], Constantin Koch[1], Indrani Dey[1], Frederic Ussling[1], Linos Hecht[1], Yves Acremann[1], Isabelle Bollier[1], Alessandro Colombo[1], Ehsan Hassanpour[1], Katharina Kolatzki[1], Changji Pan[1], Mario Sauppe[1], Lea Schüpke[1], Björn Senfftleben[1], Hanchao Tang[2], Arnab Choudhury[2], Bruce Yoder[2], Ruth Signorell[2], and Daniela Rupp[1] — [1]D-PHYS, ETH Zürich — [2]D-CHAB, ETH Zürich

Homogeneous freezing of free-flying water droplets of 1μm radius and smaller remains largely not understood due to the resolution limit of optical imaging. A change in freezing dynamics is expected in respect to droplets over 10μm [1], but no experimental study has confirmed this. Ice nucleation rates are also uncertain, with previous studies not agreeing on a compatible value [2]. Using intense XUV pulses from our tabletop HHG source, we obtain single-shot diffraction patterns of individual nanodroplets injected using an aerodynamic lens, to investigate possible morphology changes related to freezing. Here, the first results from this measurement are shown.

[1] Buttersack, T et al., JPCB 120 (2016): 504

[2] Amaya, A. and Wyslouzil, B., J. Chem. Phys. 148.8 (2018)

MO 21.8 Wed 17:00 Philo 1. OG

High-Resolution Electron Spectroscopy of Doped Helium Nanodroplets with a Hemispherical Electron Analyzer — •Narcis-Silviu Blaj[1], Niklas Scheel[2], Rajni Rajni[1], Asbjørn Laegdsmand[1], Aleksandar Milosavljevic[3], John Bozek[3], and Marcel Mudrich[1,2] — [1]Institute of Physics, University of Kassel, D-34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [3]Soleil Synchrotron, 91190 Saint-Aubin, France

Helium nanodroplets (HNDs) have mostly been used as inert cryomatrices for spectroscopy of embedded molecules and clusters.

We performed the first high-resolution X-ray photoelectron spectroscopy (XPS) measurements of pure and doped helium nanodroplets at the PLEIADES beamline of SOLEIL Synchrotron using a hemispherical electron analyzer (HEA). In particular, we explored droplets doped with krypton and argon. The formation of Ar and Kr clusters was identified through the appearance of additional low-binding-energy features accompanying the spin-orbit doublets of the atomic photolines (Kr 3d and Ar 2p), in agreement with earlier observations of photoemission from pure small Kr and Ar clusters. We systematically recorded XPS spectra as a function of photon energy, droplet size, and doping level, allowing us to study the evolution of spectral line shifts and intensity ratios between atomic and cluster-specific components.

In addition, we plan further experiments at SOLEIL as well as at other synchrotron facilities to explore a wider range of photon energies, dopants, and cluster conditions.

MO 22: Poster – Cold Molecules (joint session MO/Q)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

MO 22.1 Wed 17:00 Philo 1. OG

Progress on Zeeman slowing CaF — •Julius Niederstucke, Timo Poll, Paul Kaebert, Sebastian Anskeit, Mirco Sierke, and Silke Ospelkaus — Leibniz Uni Hannover

Significant advancements have recently been achieved in direct laser cooling of molecules, bringing them to temperatures near absolute zero [1, 2]. However, the number of molecules that can be captured from molecular beams using conventional laser cooling methods remains a limiting factor in such experiments [3, 4]. In this work, we present strategies to enhance the yield of molecules in such experiments. To this end, we present our experimental findings on the Zeeman slower developed for directly laser-coolable molecules, as proposed by our group [5], and outline the initial steps towards creating a sub-Doppler engineered red magneto-optical trap [6,7]. [1] J. F. Barry et al. 2012 [2] Y. Wu et al. 2021 [3] S. Truppe et al. 2017 [4] L. Anderegg et al. 2017 [5] M. Petzold et al. 2018 [6] S. Xu et al. 2021 [7] S. Xu et al. 2022

MO 22.2 Wed 17:00 Philo 1. OG

Towards laser cooling of NH radical — •Ashish Mahangare, Daniel Roesch, and Edvardas Narevicius — TU Dortmund, Germany

Ultra-cold molecules open up a wide variety of applications like quantum control, ultra-cold chemical dynamics, quantum information, tests of fundamental constants and precision measurements. Laser cooling has been applied for a few diatomic molecules such as SrF, CaF and YO, YbF, AlF, BaF and a poly-atomic molecule CaOH.

Our goal is to laser cool ^{15}NH. The main transition of interest for laser cooling is $(X^3\Sigma^-)(v" = 0, N" = 1, J" = 1)$ to $A^3\Pi(v' = 0, N' = 1, J' = 0)$ at 336 nm. The excited state of this cooling transition has a lifetime of around 400 ns. This electronic transition is rotationally closed and has highly diagonal FCFs.

We performed laser-induced fluorescence (LIF) to study the hyperfine structure of laser cooling transition. I will also present Terahertz rotational spectroscopy to pump molecules from N = 0 to N =1 state. Terahertz spectroscopy is also performed to get highly precise hyperfine splitting in N = 0 and N = 1 rotational states for $X^3\Sigma^-$.

MO 22.3 Wed 17:00 Philo 1. OG

Collisions in a quantum gas of bosonic ^{23}Na^{39}K molecules — •Fritz von Gierke[1], Mara Meyer zum Alten Borgloh[1], Jule Heier[1], Philipp Gersema[1], Kai Konrad Voges[2], Baraa Shammout[1], Eberhard Tiemann[1], Leon Karpa[1], and Silke Ospelkaus[1] — [1]Institut für Quantenoptik, Leibniz Universität Hannover — [2]Centre for Cold Matter, Blackett Laboratory, Imperial College London

We present our latest experimental results on ultracold NaK quantum gases, focusing on atom-molecule and molecule-molecule collisions. In particular, we report recent advances in the electric field control of atom-molecule Feshbach resonances and shielding of collisions with implications for future quantum simulations and many-body physics.

MO 22.4 Wed 17:00 Philo 1. OG

Crystal-to-droplet melting in ultracold polar molecules — •William Freitas, Panagiotis Giannakeas, and Jan M Rost — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Microwave-shielded polar molecules provide a novel platform for exploring dipolar matter in the strongly correlated regime, where dipole-dipole interactions naturally confine molecular ensembles to quasi-two-dimensional geometries. The competition between the long-range antidipolar attraction and the anisotropic short-range repulsion leads to a rich variety of phases, ranging from quantum droplets to crystalline structures.

In this work, we investigate the transition between the crystal and droplet phases, focusing specifically on the melting of crystalline order for finite systems. For systems of up to N = 40 molecules, we observe that the system develops droplet-ring configurations as an intermediate state between the droplet and crystal phases, characterized by a superfluid fraction below unity. Moreover, we show that the droplet-ring state retains six-fold symmetry, a fingerprint of the underlying crystal structure, as demonstrated by the pair-correlation function and structure factor.

Our simulations employ the Variational Monte Carlo method with a neural-network quantum state as the trial wave function. This approach provides a highly flexible functional form and enables stable energy minimization, yielding an accurate description of the ground state and an efficient treatment of strongly correlated finite systems.

MO 22.5 Wed 17:00 Philo 1. OG

Towards laser cooling of NH radical — •Ashish Mahangare, Daniel Roesch, and Edvardas Narevicius — TU Dortmund, Germany

Ultra-cold molecules open up a wide variety of applications like quantum control, ultra-cold chemical dynamics, quantum information, tests of fundamental constants and precision measurements. Laser cooling has been applied for a few diatomic molecules such as SrF, CaF and YO, YbF, AlF, BaF and a poly-atomic molecule CaOH.

Our goal is to laser cool ^{15}NH. The main transition of interest for laser cooling is $X^3\Sigma^-(v" = 0, N" = 1, J" = 1)$ to $A^3\Pi(v' = 0, N' = 1, J' = 0)$ at 336 nm. The excited state of this cooling transition has a lifetime of around 400 ns. This electronic transition is rotationally closed and has highly diagonal FCFs.

We performed laser-induced fluorescence (LIF) to study the hyperfine structure of laser cooling transition. I will also present Terahertz rotational spectroscopy to pump molecules from N = 0 to N =1 state. Terahertz spectroscopy is also performed to get highly precise hyperfine splitting in N = 0 and N = 1 rotational states for $X^3\Sigma^-$.

MO 23: Contributions to SYLC I

Time: Thursday 11:00–12:45 Location: P 110

Invited Talk MO 23.1 Thu 11:00 P 110

Large circular dichroism in the total photoemission yield of free chiral nanoparticles created by a pure electric dipole effect — •Sebastian Hartweg[1,2], Dušan K. Božanić[3], Gustavo A. Garcia-Macias[2], and Laurent Nahon[2] — [1]Institute of Physics, University of Freiburg, Germany — [2]Synchrotron Soleil, St. Aubin, France — [3]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Spectroscopic techniques that are sensitive to molecular chirality are important analytical tools to quantitatively determine enantiomeric excess and purity of chiral molecular samples. Many chiroptical processes however produce weak enantio-specific asymmetries due to their origin relying on weak magnetic dipole or electric quadrupole effects. Photoelectron circular dichroism (PECD) in contrast, is an intense effect, that is fully contained in the electric dipole description of light matter interaction and creates a chiral asymmetry in the photoelectron angular distribution. Here, we demonstrate that this chiral signature in the angular distribution of emitted electrons can be translated into the total photoionization yield for submicron-sized condensed samples. The resulting chiral asymmetry of the photoionization yield (CAPY), mediated by the attenuation of light within the particles, can be detected experimentally without requiring high vacuum systems and electron spectrometers. This effect can be exploited as an analytical tool with high sensitivity to chirality and enantiopurity for studies of chiral organic and hybrid submicron particles in environmental, biomedical or catalytic applications.

MO 23.2 Thu 11:30 P 110

Investigating transient localized charges in small chiral molecules with free-electron lasers — •Markus Ilchen on behalf of a large collaboration — University of Hamburg, Germany — Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — European XFEL, Schenefeld, Germany

Chirality, the inherent "handedness" of many molecular structures, is a cornerstone of biological processes, influencing and steering interactions at the molecular level as well as shaping a broad variety of the physical and chemical properties of matter. The technological evolution of free-electron lasers will be presented in terms of polarization control and high-power attosecond pulse generation in the soft X-ray regime, which enables them to create and explore transiently chiral systems with localized charges at the onset of structural dynamics. This opens the new field of site-specific investigations of building blocks of life at the onset of dynamics outside of the nucleus.

MO 23.3 Thu 11:45 P 110

Correlation between Circular Dichroism and Chirality-Induced Spin Selectivity — •Raoul M. M. Ebeling[1], Maurice Béringuier[1], Vladimiro Mujica[2], Daniel M. Reich[1], and Christiane P. Koch[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Arizona State University, Arizona, United States of America

We investigate whether absorption circular dichroism (CD) and chirality-induced spin selectivity (CISS) share common physical origins in the interaction of chiral molecules with circularly polarized light. Using a one-electron model in which an effective chiral potential mimics a chiral molecule, we analyze how the chiral potential and spin-orbit coupling strength influence CD and CISS, respectively. We find that the CD signal increases with the chiral potential strength and decreases with stronger spin-orbit coupling. The difference in spin polarization shows a more complex behavior, and we surprisingly find that strong spin-orbit coupling or strong chiral potentials reduce its value. This is caused by the corresponding Hamiltonian terms diminishing the effect of the other, a trend clearly reflected in the energy scales of the competing interactions. Consequently, the strongest enantiomer-sensitivity of the spin polarization is obtained when balancing the two. Lastly, we observe a correlation between CD and CISS that becomes weaker for strong chiral potentials.

MO 23.4 Thu 12:00 P 110

Non-Dichroic Enantio-Sensitive Chiroptical Spectroscopy — Letizia Fede[1], Debobrata Rajak[2], Chris Sparling[3], David Ayuso[4], Valérie Blanchet[1], Piero Decleva[5], Dominique Descamps[1], Stéphane Petit[1], Bernard Pons[1], Yann Mairesse[1], and •Andrés Ordóñez[6] — [1]Université de Bordeaux CNRS CEA CELIA, France — [2]ELI ALPS, Hungary — [3]Heriot-Watt University, UK — [4]Imperial College London, UK — [5]Università degli Studi di Trieste, Italy — [6]Freie Universität Berlin, Germany

Chiroptical effects using circularly polarized light produce signals that change sign when switching either molecular handedness (enantiosensitivity) or light helicity (circular dichroism). Here, we break this enantiosensitive-and-dichroic paradigm by measuring a new type of chiroptical signal which is enantiosensitive but not dichroic. We photoionize chiral molecules using a strong laser field and detect the three-dimensional photoelectron momentum distribution (PMD). The Non-Dichroic, Enantio-Sensitive asymmetry is encoded in octupolar and higher multipolar terms in the PMD, appearing in multiphoton ionization with elliptical or cross-polarized two-color fields. Our simulations agree with our measurements and show that this effect extends from the two-photon to the strong-field ionization regime. The robustness of the enantiosensitivity with respect to the relative phase between the orthogonal components of the ionizing field represents an example of symmetry protection, opening unexplored opportunities for imaging ultrafast dynamics in chiral molecules, such as enantiosensitive photoelectron spectroscopy with bright squeezed vacuum states.

MO 23.5 Thu 12:15 P 110

Femtosecond transient circular dichroism spectroscopy of chiral organic-inorganic lead perovskites — •Thomas Lenzer and Kawon Oum — University of Siegen, Physical Chemistry 2, Adolf-Reichwein-Str. 2, 57076 Siegen

Chiral lead-based perovskites represent promising candidates for the generation of spin-polarized charge carriers, enabling advances in spintronic and optoelectronic applications. We report thin films of hybrid organic-inorganic perovskites that exhibit pronounced circular dichroism (CD) responses reaching 5000 mdeg and dissymmetry factors exceeding 0.10, with negligible contributions from linear dichroism and linear birefringence. Using transient circular dichroism (TrCD) spectroscopy with femtosecond resolution,[1,2] we investigate the ultrafast dynamics of spin-polarized carriers. Complementary transient absorption measurements reveal the dominant relaxation pathways following photoexcitation in these materials.

[1] D. Gust, M. Scholz, V. Schumacher, J.-C. Mulatier, D. Pitrat, L. Guy, K. Oum and T. Lenzer, Sci. Rep. 2024, 14, 12694. [2] M. Morgenroth, M. Scholz, M. J. Cho, D. H. Choi, K. Oum and T. Lenzer, Nat. Commun. 2022, 13, 210.

MO 23.6 Thu 12:30 P 110

Ultra-fast nonlinear optical response of chiral molecules with a focus on conformer sensitivity — •Elena Aethra Christou[1,3], David Ayuso[2], Felipe Morales[1], and Olga Smirnova[1,3] — [1]Max Born Institute, Berlin, 12489, Germany — [2]Imperial College London, SW7 2AZ,UK — [3]Technische Universität Berlin, 10623, Germany

We model the ultrafast nonlinear response of chiral molecules using TDDFT and temporally and spatially confined, CEP-controlled linearly polarized pulses. Focusing generates a longitudinal field component that produces forward elliptically polarized light, which in turn drives a chiral response orthogonal to the propagation plane, leading to even-harmonic emission. Interference between achiral odd and chiral even harmonics, shaped by the CEP, yields enantio-sensitive optical rotation. Building on previous work demonstrating this, we extend this approach to investigate the interplay between electronic dynamics and molecular conformations. We apply this mechanism to the three most abundant conformers of the chiral amino acid serine, which have reported gas-phase populations of 43.7%, 18.8%, and 14.8%. Their distinct polarization signatures are quantified through molecular QR codes that encode conformer-dependent chiral dynamics. These differences reveal a clear conformer-specific chiral response. The approach demonstrates the potential of CEP-controlled fields for conformer-resolved chiral spectroscopy in the near-infrared regime.

MO 24: Molecular Spectroscopy I

Time: Thursday 11:00–12:45 Location: P 204

Invited Talk MO 24.1 Thu 11:00 P 204

Electronic Spectra of Doped Diamondoid Cations — •Parker Crandall, Ronja Schramm, Sebastian Völz, Domenik Schleier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

Pre-solar nanodiamonds grains have been found in significant abundance in primitive carbonaceous chondrites, suggesting a possible interstellar origin. Their presence raises the question of whether aliphatic (sp^3-hybridized), diamond-like hydrocarbons can form and survive in the harsh conditions of the interstellar medium. Diamondoid cations represent compelling spectroscopic targets. Not only are diamondoids the smallest molecular units of bulk diamond, but their cations are relatively stable and have electronic transitions that lie in the visible range, making them potential candidates as carriers of the diffuse interstellar bands. While our previous work focused on bare and functionalized derivatives, we present our recently measured spectra of N-, O-, and S-doped (cage-modified) diamondoid cations, measured in the gas-phase using either a photoelectron spectrometer, a cryogenically cooled ion trap coupled to a tandem mass spectrometer, or both. These results are further supported by quantum chemical calculations and can provide critical reference data for astronomical searches in the pursuit of a broader understanding of the chemical inventory of the interstellar medium.

MO 24.2 Thu 11:30 P 204

The first excited state of OH^+He — •Nima-Noah Nahvi and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The OH^+He dimer serves as a simple system to study the weak interaction of helium with open-shell cations, relevant to microscopic superfluidity and astrochemistry. In this work, we investigate the first excited state of OH^+He using a combined spectroscopic and computational approach. Quantum chemical calculations suggest that the transition into this state exhibits an unusual proton transfer to the helium atom ($OH^+ \cdots He \to O \cdots H^+He$). To prove this, we generate OH^+He inside a cryogenic quadrupole ion trap (10 K) and irradiate the clusters with tunable UV laser light to induce photodissociation. By detecting the dissociation fragments with a time-of-flight mass spectrometer, we obtain an optical action spectrum and are able to directly observe the proton transfer. Calculated potential energy surfaces of the ground and excited state at the coupled cluster level support our interpretation. In addition, we numerically calculate the vibrational wavefunctions, which give insights into the spectrum and the vibrational dynamics of the dissociation process into HeH^+.

MO 24.3 Thu 11:45 P 204

Towards Light-Shift Spectroscopy of RbYb near the D1 line of Rb — •Céline Castor — Institut für Experimentalphysik, Heinrich-Heine-Universität Düsseldorf

Ultracold dipolar molecules constitute a promising system for the investigation of topics like ultracold chemistry, novel interactions in quantum gases, precision measurements and quantum information.

Here we report on experiments in our apparatus for the production of ultracold RbYb molecules. In our former setup photoassociation experiments near the D1 line of Rb were conducted. Our current setup constitutes an improvement of our old apparatus, where the interactions in RbYb and possible routes to molecule production have already been studied extensively, including two-photon photoassociation spectroscopy near the Yb intercombination line.

A major goal is the efficient production of ground state RbYb molecules. We employ optical dipole traps to transport individually cooled samples of Rb and Yb from their separate production chambers to a dedicated science chamber. Combining our results on photoassociation spectroscopy near the Rb D1 line and the Yb intercombination line, we present a conceptual approach for studying stronger bound states in the excited molecular potential $^2\Pi_{1/2}$ using light-shift spectroscopy.

MO 24.4 Thu 12:00 P 204

Shedding Light on $(SiC)^+_{1,2}$: First Laboratory Spectra Obtained by Electronic Photodissociation — •Kai Pollow, Alexander Breier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

Silicon carbide ions ($Si_nC_m^+$) are expected in carbon-rich circumstellar environments such as those around asymptotic giant branch stars[1,2]. Several small neutral Si_nC_m species are known in the interstellar medium[3], but their cations remain unidentified due to missing spectroscopic data[4]. Spectra of $Si_nC_m^+$ are therefore essential for assessing their role in ion–molecule chemistry and silicon carbide dust formation.

We present the first laboratory spectra of $(SiC)^+_{1,2}$, recorded via vibronic photodissociation of mass-selected ions in a quadrupole/time-of-flight tandem mass spectrometer with a laser vaporization source[4]. The spectra exhibit clear vibrational structure, and the derived parameters agree with quantum-chemical predictions.

References:
[1] T. Chen et al., Mon. Not. R. Astron. Soc. 509, 5231 (2022).
[2] M. C. McCarthy et al., J. Mol. Spectrosc. 356, 7 (2019).
[3] S. Massalkhi et al., Astron. Astrophys. 611, A29 (2018).
[4] M. Förstel et al., J. Mol. Spectrosc. 377, 111427 (2021).

MO 24.5 Thu 12:15 P 204

Orbital-Resolved Bond-Breaking Asymmetry in the Strong-Field Dissociative Double Ionization Channel ($N_2^+ + O^+$) of N_2O — •Feras Afaneh — Physics Department, Faculty of Science, Hashemite University, P.O.Box 330127, Zarqa 13133, JORDAN

The dissociative double ionization of nitrous oxide (N_2O), induced by short-pulse polarized laser fields, was investigated using the COLTRIMS technique. Focusing on the dissociative channel ($N_2^+ + O^+$), we extracted both the molecular-frame photoelectron angular distributions and the ion sum-momentum distributions. Orientation-dependent ionization rates, analyzed across distinct kinetic energy release (KER) regimes, revealed contributions from multiple molecular orbitals. These results reveal a pronounced asymmetry in bond breaking relative to the instantaneous laser field vector, arising from the interplay between orbital geometry and electron localization-assisted enhanced ionization in stretched molecular configurations under strong-field conditions.

MO 24.6 Thu 12:30 P 204

Photoelectron Spectroscopy and dissociative photoionization of nitrogen heterocycles — •Domenik Schleier[1], Jordy Bouwman[2], Helgi Hrodmarsson[3], Andras Boedi[4], Patrick Hemberger[4], and Otto Dopfer[1] — [1]Institut für Physik und Astronomie, TU Berlin, Germany — [2]Department of Chemistry, CU Boulder, USA — [3]Laboratoire Inter-Universitaire des Systèmes Atmosphérique, Paris, France — [4]Paul-Scherrer-Institute, Villigen, Switzerland

Polycyclic aromatic hydrocarbons (PAHs) and their nitrogen-containing counterparts (PANHs) are ubiquitous in extraterrestrial environments ranging from planetary atmospheres to the interstellar medium. However, only large PA(N)Hs survive the extreme conditions, whereas smaller ones are destroyed. In this work, three nitrogen-containing PANH isomers of C8H6N2 composition have been studied by mass-selected threshold photoelectron spectroscopy and dissociative photoionization in a double imaging photoelectron photoion coincidence (i2PEPICO) apparatus at the VUV beamline of the Swiss Light Source. The experimental findings are supported by quantum chemical calculations and energy-dependent unimolecular dissociation rates for each channel were calculated as a function of internal energy based on RRKM statistical rate theory. The isomers show characteristic dissociation pathways that lead to the elimination of HCN, N2 and H fragments depending on the relative nitrogen position.

MO 25: Molecular Collisions and Kinetics

Time: Thursday 14:30–15:15 Location: P 105

MO 25.1 Thu 14:30 P 105

Mutual neutralization reactions in a cryogenic ion trap — •Maximilian Märk, Michael Hauck, Robert Wild, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

While there are many studies on ion-neutral reactions at low temperatures, mutual neutralization (MN) reactions are still experimentally poorly understood. However, these anion-cation reactions play a crucial role in the astrochemical models of interstellar clouds [T. J. Millar *et al.*, Chem. Rev. 117, (2017)]. In the literature the majority of these reactions are assigned the same rate coefficient, which is an approximation [N. S. Shuman *et al.*, J. Phys.: Conf. Ser. 300 (2011)]. We will address this gap by measuring MN reactions for abundant ions in interstellar space. To achieve this, we will utilize our cryogenic 16-pole wire trap, which is designed to create a relatively flat potential with steep walls [M. Nötzold *et al.*, Phys. Rev. A, 106 (2022)]. The wires of the trap are driven with an RF voltage to contain the ions radially. A DC voltage is usually applied to endcap electrodes for axial confinement, but this only works for one charge polarity at a time. To perform MN reactions, we will also drive the axial confinement using an RF voltage. The large expected cross section due to the attractive Coulomb potential will be offset by the low densities in the ion trap. Therefore, long storage times are essential. Our group has already demonstrated long trapping lifetimes for three-body reaction studies [C. Lochmann *et al.*, J. Phys. Chem. A, 127 (2023)]. Our measurements will provide much-needed data for astrochemical models.

MO 25.2 Thu 14:45 P 105

Gas phase redox stability of the molecular ruby [Cr(ddpd)2]3+ and related complexes — •Boris Heeb, Jana Eck, and Jennifer Meyer — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

Chromium(III) complexes, also known as molecular rubies, exhibit particularly good luminescence properties.[1,2] Studies on gas phase stability of these compounds are rare to date. For this reason, the stability of the chromium complexes $[Cr(ddpd)_2]^{3+}$ (ddpd=N,N′-dimethyl-N,N′-dipyridin-2-ylpyridine-2,6-diamine), $[Cr(bpmp)_2]^{3+}$ (bpmp=2,6-bis(2-pyridylmethyl)pyridine), and $[Cr(tpeF)_2]^{3+}$ (tpeF=singly fluorinated 1,1,1-tris(pyrid-2-yl)ethane) with the corresponding reduced forms were examined in the gas phase through collision-induced dissociation. The experiments were performed on an electrospray ionization quadrupole mass spectrometer with in-situ reduction. Quantum chemical calculations suggest that $[Cr(ddpd)_2]^{3+}$ undergoes a metal-centered transition upon photoexcitation, whereas $[Cr(tpe)_2]^{3+}$ undergoes a ligand-centered transition.[3] However, fragmentation patterns of the reduced complexes show strong similarities, whereas the triply-charged complexes show different fragmentation behavior. In contrast, a different pattern can be observed for $[Cr(bpmp)_2]^{3+}$, which is assigned a mixed behaviour in condensed phase.

[1] W. R. Kitzmann et al., *Dalton Trans.* **2022**, *51*, 6519-6525. [2] F. Reichenauer et al., *J. Am. Chem. Soc.* **2021**, *143*, 11843-11855. [3] S. Otto et al., *Angew. Chem. Int. Ed.* **2015**, *54*, 11572-11576.

MO 25.3 Thu 15:00 P 105

Investigating electron and proton transfer reactions with velocity map imaging — •Viviane C. Schmidt, Dasarath Swaraj, Jerin Judy, Fabio Zappa, and Roland Wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Crossed-beam apparatuses employing velocity map imaging (VMI) techniques are versatile tools to study ion-neutral collisions. Here, it is possible to either directly measure or infer the kinematics of all reactants and products, enabling a detailed look into underlying reaction mechanisms. These include the transfer of charge, either in the form of an electron or a proton, from one species to the other.

Two prototypical systems will be discussed here. The first reaction is the electron transfer between Ar^+ and N_2 studied at the newly-commissioned crossed-beam apparatus at Innsbruck University [1]. Here, it was possible to measure the reaction pathway into the N_2^+ vibrational ground state at low collision energies. It showed clear signatures of complex-mediated dynamics.

The second reaction is the proton transfer between HeH^+ and H_2. Here, a special focus is placed on the influence of rotational excitation of the charged reactant. For this project, a technical upgrade of a second crossed-beam set-up at Innsbruck University is ongoing. The current status as well as next steps will be presented.

[1] D. Swaraj *et al.*, in preparation

MO 26: Contributions to SYLC II

Time: Thursday 14:30–16:15 Location: P 110

Invited Talk MO 26.1 Thu 14:30 P 110

Differentiating Between Enantiomers with Nuclear Quadrupole Coupling Using Microwave Three-Wave Mixing — •Freya E. L. Berggötz[1,2], Monika Leibscher[3], Wenhao Sun[1], Christiane P. Koch[3], and Melanie Schnell[1,4] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany — [3]FU Berlin, Fachbereich Physik and Dahlem Center for Complex Quantum Systems, Berlin, Germany — [4]Institut für Physikalische Chemie, CAU zu Kiel, Kiel, Germany

We demonstrate the application of microwave three-wave mixing to the amino alcohol valinol, which displays a hyperfine structure in the rotational spectrum due to nuclear quadrupole coupling. The hyperfine structure complicates the typical triad of rotational states, leading to overlapping microwave three-wave mixing cycles. We identified a set of cycles accessible within the hyperfine substructure of the rotational states $|J_{K_aK_c}\rangle = |1_{01}\rangle, |2_{12}\rangle$, and $|2_{02}\rangle$ by applying the selection rules for rotational transitions and nuclear quadrupole coupling. To address an individual cycle of hyperfine transitions or subsets of cycles simultaneously, we explored different pulse schemes exploiting single-frequency or chirped microwave pulses. Each pulse scheme generated a distinct chiral signal, which shows clear enantiomer differentiation. The experimental findings agree very well with numerical simulations using an effective model for the hyperfine interaction. This study thus extends the applicability of microwave three-wave mixing to previously unexplored molecular systems containing quadrupolar nuclei.

MO 26.2 Thu 15:00 P 110

Dynamical chirality in rotating molecules induced by electron transitions — •Marjan Mirahmadi[1], Alexander Gabriel Löhr[1], Andres Felipe Ordonez[2,3], and Olga Smirnova[1,4] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [2]Department of Physics, Imperial College London, SW7 2BW London, United Kingdom — [3]Department of Physics, Freie Universit\"at Berlin, 14195 Berlin, Germany — [4]Technische Universität Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

Although chirality is typically considered a spatial property of an object and depends on its geometrical symmetries such as point inversion and reflection, local chirality arises from a vector tracing a chiral trajectory in time. For instance, locally chiral Lissajous figures of light are known to generate strong enantiosensitive signals in HHG. Inspired by this concept, we introduce locally chiral molecular rotations via rotational wavepackets constructed of few lower rotational states, in contrast to previously demonstrated rotational chirality by using an optical centrifuge.

We then explore the interplay of two locally chiral structures: the induced polarization vector of chiral electron currents and the rotational trajectory of a molecule, both driven by locally chiral fields. We formally investigate how controlled molecular rotation affects the electronic excitations in different ultrafast electronic process. Moreover, including the electron-rotational couplings based on Hund's cases (a) and (b), we provide deeper insight into how electronic currents effect this newly introduced form of rotational chirality.

MO 26.3 Thu 15:15 P 110

Induced Photoelectron Circular Dichroism onto an Achiral Chromophore — •Etienne Rouquet[1,2], Madhusree Roy Chowdhury[1], Gustavo Garcia[1], Laurent Nahon[1], Jennifer Dupont[2], Valéria Lepère[2], Katia Le Barbu-Debus[2], Rodolphe Vuilleumier[3], and Anne Zehnacker[2] — [1]Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, F-91190 St Aubin, France — [2]Institut des Sciences Moléculaires d*Orsay (ISMO), CNRS, Université Paris-Saclay, F-91405 Orsay, France — [3]Chimie Physique et Chimie du vivant (CPCV), École Normale Supérieure, Sorbonne Université, CNRS 75005 Paris, France

For the first time, we recorded induced photoelectron circular dichroism (PECD). More specifically, we formed molecular complexes in the gas phase, separated in two moieties. One part is chiral, but does not have a chromophore, and the other is a non-chiral moiety with a chromophore. We recorded induced PECD of the phenol-methyloxirane (Phe-MOx) complex using VUV synchrotron radiation. The HOMO is localized solely on the phenol moiety and we saw a non-zero chiroptical response originating from the ionization of the complex, which we first assigned to the electron scattering off the chiral molecular potential. We then successfully applied this technique using a ns-laser 2 photon energy scheme, providing conformer-selective PECD data. We confirmed our synchrotron-based results on conformer-selected Phe-MOx molecular complexes, with two structures observed in the gas phase. Hydrogen bonding with both lone pairs of the MOx oxygen atom were involved, revealing a chiral deformation of the phenol.

MO 26.4 Thu 15:30 P 110

Enantioselctive Occupation Transfer via Berry Phase Cycling — •Aycke Roos[1], Pablo Maier[1], and Olga Smirnova[1,2] — [1]Max-Born-Institut — [2]Technische Universität Berlin

A chiral molecule interacting with synthetic chiral light acquires geometric properties as the Lissajous figure of this light is adiabatically deformed in a cycle. During this cycle the electronic wave function of the molecule acquires a geometric (Berry) phase.

The phase serves as the fundamental quantity that encapsulates the geometric interplay between field and molecule. It naturally provides a clear geometric picture stripped from any dynamical processes. It further enables the identification of explicit polarization protocols to maximize the enantioselective excitation of one of one enantiomers. In particular, we find that a reversal of the temporal polarization vector trajectory quantified by the winding number leads to a switch between preferential excitation of left-or right handed molecules.

MO 26.5 Thu 15:45 P 110

Enantiosensitive Chern Numbers in Chiral Molecules Driven by Synthetic Chiral Light — •Pablo Maier[1], Aycke Roos[1], and Olga Smirnova[1,2] — [1]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Straße 2A, 12489 Berlin, Germany — [2]Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Temporal geometry describes ultrafast chiral dynamics in molecules by showing how light-driven electronic currents depend on molecular orientation. In our driving scheme the electronic response is effectively independent of one Euler angle, so the relevant orientation space reduces to a sphere parametrized by two angles. The driven electronic states then form smooth bands over this sphere, characterized by a Berry connection, Berry curvature, and associated topological invariants. We show that these orientation-space bands can carry integer-quantized, enantio-sensitive Chern numbers. In a driven three-level electronic manifold used as a minimal model, the dressed eigenstates define three non-degenerate bands whose Chern numbers always sum to zero but are individually nonzero and reverse sign upon exchanging enantiomers. By varying detunings and field parameters, we locate band-touching points where gaps close and the band Chern numbers jump by integer amounts, signaling topological phase transitions between distinct chiral phases.

MO 26.6 Thu 16:00 P 110

Optimising enantioselective electronic population transfer in chiral molecules — •Daniel García González and Andrés Ordóñez — Department of Physics, Freie Universität Berlin, Berlin, Germany

Coherent control offers powerful routes to all-optical enantioselective photochemistry. Our approach is based on electronic transitions, requires neither cold molecules nor intermediate resonances nor chiral sensitisers, and is applicable to randomly oriented molecules. Strong ($> 10\%$) population differences in opposite enantiomers arise from the interference between two multiphoton excitation pathways driven by a fundamental IR field and two of its harmonics.

In this regime, the population difference takes the form [arXiv:2309.02392v2]

$$P_R - P_S \propto \mathrm{Re}\left[\mathbf{g}^{(5)} \cdot \mathbf{h}^{(5)}\right],$$

where $\mathbf{g}^{(5)}$ encodes the molecular geometry, while $\mathbf{h}^{(5)}$ depends on the polarizations of the applied fields and is experimentally controllable.

We study the dependence of $\mathbf{g}^{(5)}$ on the molecular structure using the three conformers of carvone, and introduce a strategy to design polarisation schemes that maximise $\mathrm{Re}[\mathbf{g}^{(5)} \cdot \mathbf{h}^{(5)}]$. This approach yields experimentally realistic field configurations achieving enantioselective population differences of up to 55% -nearly twice the previously reported 30%- offering a clear, geometry-based method for optimising coherent enantioselective control in electronic transitions.

MO 27: Molecular Spectroscopy II

Time: Thursday 14:30–16:30 Location: P 204

MO 27.1 Thu 14:30 P 204

Photoswitchable Nanoparticle Arrays — •Heyou Zhang[1], Pankaj Dharpure[1], Paul Mulvaney[2], Mukundan Thelakkat[1], and Jürgen Köhler[1] — [1]University of Bayreuth — [2]University of Melbourne

Recent advancements in nanophotonics have significantly enhanced optical data storage and display technologies by enabling dynamic control of light emission. A key challenge in this field is achieving precise manipulation of material emission properties at micro to nano scales on solid-state substrates. To address this challenge, we introduce Surface-Templated Electrophoretic Deposition (STEPD) for fabricating arrays of polymer beads incorporating photo-switchable diarylethene (DAE) molecules. This method allows the creation of well-ordered arrays, enabling selective optical addressing of individual beads to modulate their emission states (on/off) at micrometer scale. Our research explores binary data processing capabilities through selective writing, reading, and erasing operations within specific photonic units. These findings demonstrate the feasibility of continuous recording, opening new possibilities for advanced optical memory devices in optoelectronic systems.

MO 27.2 Thu 14:45 P 204

First Observation of Resonant Auger-Driven Intermolecular Coulombic Decay in Aqueous Solutions — •Dana Bloss[1], Rémi Dupuy[2], Florian Trinter[3], Noelle Walsh[4], Gunnar Öhrall[4], Niklas Golchert[1], Gabriel Klassen[1], Adrian Krone[1], Yusaku Terao[1], Johannes H. Viehmann[1], Lorenz S. Cederbaum[5], Uwe Hergenhahn[3], Olle Björneholm[6], Arno Ehresmann[1], and Andreas Hans[1] — [1]Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Laboratoire de Chimie Physique - Matière et Rayonnement, CNRS, LCP-MR, Sorbonne Université — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [4]MAX IV Laboratory, Lund University, Box 118, 22100 Lund, Sweden — [5]Theoretische Chemie, Institut für Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany — [6]Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden

Over the last decades, non-local ionization mechanisms such as interatomic Coulomb decay (ICD) have attracted considerable interest, primarily due to their potential significance for radiation biology. Here, we report the first experimental observation of resonant Auger decay-induced ICD (RA-ICD) in a liquid environment. The process was identified in solvated Ca ions using a combination of high-resolution and coincident electron spectroscopy on liquid microbeams. RA-ICD enables the site-specific and energy-specific generation of low-energy electrons, which are known for their genotoxicity.

MO 27.3 Thu 15:00 P 204

Low temperature ultraviolet photodissociation spectroscopy of $[\text{dAMP-H}]^-$ — •Christian Sprenger[1], Samuel J. M. White[1], Miriam Westermeier[1], Gabriel Schöpfer[1], Franziska Dahlmann[1,3], Uma Namangalam[2], Salvi Mohandas[2], Sunil Kumar S.[2], Eric S. Endres[1], and Roland Wester[1] — [1]Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria — [2]Indian Institute of Science Education and Research Tirupati, Department of Physics, Panguru, Andhra Pradesh, India - 517619 — [3]Current address: Department of Chemaical Engineering, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden

To deepen the understanding of photoexcitation of DNA by ultraviolet radiation, we performed a wavelength dependent photoabsorption study of the anionic deprotonated nucleotide $[\text{dAMP-H}]^-$. Within the range of our study, between 240 nm and 270 nm, we were able to resolve multiple spectral features, that could not be resolved before. This was made possible by our 16-pole radiofrequency wire trap, which operates at a temperature of 3 K. Furthermore, we analysed the yield of five ionic photofragments as a function of wavelength. Finally we determined the absolute photofragmentation cross section of $[\text{dAMP-H}]^-$, by performing a comparative measurement of the I^- photodetachment cross section. The results of these photodissociation measurements, published in Ref [1], will be presented.

[1] C. Sprenger et al., *J. Phys. Chem. A*, (in press)

MO 27.4 Thu 15:15 P 204

Dissociative Single and Double Ionization of Thymine — •Sitanath Mondal[1], Sitanath Mondal[1], Sitanath Mondal[2], Sitanath Mondal[2], Sitanath Mondal[1], and Sitanath Mondal[1]

— [1]Institute of Physics, University of Freiburg, Germany — [2]Desirs Beamline, Synchrotron Soleil, St. Aubin, France

Radiation damage on biological materials including DNA and RNA is an important research topic. Electron-Ion coincidence studies of biomolecules in gas phase can give insight about the energetics of dissociative ionization processes. While the single ionization and corresponding fragmentation has been studied previously in detail, fewer details are known about dissociative double ionization processes. I will present an electron-ion-ion coincidence study of the single and double ionization of thymine at 36 eV. The electron-ion multi-coincidence detection provided by the DELICIOUS III spectrometer at the DESIRS beamline of Soleil synchrotron enables us to retrieve detailed information on dissociative double ionization channels, including the fragment ion momentum distributions and photoelectron images of selected double ionization channels. We find pronounced differences between the dissociation channels we observe, and those previously reported for single valence shell and core level ionization, with a multitude of possible dissociation pathways accessible at this comparably low excess energy.

MO 27.5 Thu 15:30 P 204

The magnetic hyperfine structure of 1-indanol — •Kilian Hügel[1,2], JuHyeon Lee[1], Shilpa Yadav[1], Sejun An[1], Boris G. Sartakov[1], Gerard Meijer[1], and Sandra Eibenberger-Arias[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin 14195, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany

Hyperfine interactions in molecules lead to small splittings of the energy levels due to various coupling mechanisms [1]. Studying such interactions is useful for example in the investigation of molecular geometries and for the design of quantum control experiments.

In our group, we are interested in the hyperfine structure of 1-indanol since it is the target molecule in our enantiomer-specific state transfer (ESST) experiments enabling quantum control of chiral molecules [2,3]. To investigate the hyperfine structure of such a complicated molecule with ten nuclear spins, we performed UV-microwave double-resonance spectroscopy in a cold, seeded molecular beam. Additionally, we developed a theoretical model treating the nuclear spin-spin interactions leading to 672 hyperfine lines per rotational transition connected to the absolute ground state. The calculated spectra match the measurements closely, confirming the theoretical model and enabling predictions of hyperfine effects in 1-indanol.

[1] C. H. Townes and A. L. Schawlow. Microwave Spectroscopy (Dover Publications, Mineola, New York, 1975). [2] A. O. Hernandez-Castillo et al. Phys. Chem. Chem. Phys. 23, 7048-7056 (2021). [3] JH. Lee et al. Nat. Commun. 15, 7441 (2024).

MO 27.6 Thu 15:45 P 204

The Role of Nuclear Motion in Resonant Inelastixc X-ray Scattering — •Antonia Freibert[1,2], Sebastian Eckert[3], Vinicius Vaz da Cruz[3], Alexander Föhlisch[3,4], and Nils Huse[2] — [1]Department of Mathematics, Technical University of Munich, Boltzmannstraße 3, 85748 Garching b. München — [2]Department of Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [4]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

A combined theoretical and experimental study of resonant inelastic X-ray scattering (RIXS) at the nitrogen K-edge for the three diazine isomers pyrazine, pyrimidine, and pyridazine is presented. The RIXS process is simulated using fully time-dependent quantum dynamics with (multilayer) multiconfigurational time-dependent Hartree wavepacket propagation on linear vibronic-coupling Hamiltonians including up to 22 electronic states in full (24D) and reduced (6D) dimensionality. Comparison with experiment shows good agreement and reveals the strong influence of nuclear motion during the short-lived core-excited manifold on the final RIXS spectra. In particular, ultrafast non-adiabatic transitions drive symmetry-breaking distortions that give rise to additional emission bands, while interstate dynamics cause broadening and vibrational structure in the spectra. These findings provide a dynamical description of RIXS and demonstrate the importance of including nuclear motion for accurate RIXS modeling.

MO 27.7 Thu 16:00 P 204

Ultrafast dissociation dynamics of HCO$^+$ — •Anastasia Andreeva[1], Simon Reinwardt[1], Julius Schwarz[1], B. Michel Döhring[2,3], Maria Tatsch[2], David Macaluso[6], Alfred Müller[2], Nicolas Solem[5], Roland Thissen[5], Florian Trinter[4], Stefan Schippers[2,3], and Michael Martins[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]Justus-Liebig-Universität, Gießen — [3]Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt — [4]Fritz-Haber-Institut, Berlin — [5]Institut de Chimie Physique, Université Paris-Saclay, Orsay — [6]Department of Physics and Astronomy, University of Montana, Missoula

Ultrafast dissociation of molecules often results in radicals or ionic products. One of these products can be H or H$^+$, which is the key actor in many chemical reactions that rely on proton transfer. However, due to the difficulty of determining the electron densities on the atomic and femtosecond scale, the study of dissociation dynamics is experimentally difficult to achieve and requires either ultrafast pump-probe experiments or indirect investigation of dissociation products. Here we present the latter technique of obtaining information on proton dissociation after an inner-shell excitation in HCO$^+$ by resolving the kinetic energy release of the ionic fragments using the Photon-Ion Spectrometer (PIPE) at PETRA III. We used soft X-ray radiation to perform site-specific photoexcitation in HCO$^+$ and found an unexpected dissociation behavior at the C $1s \rightarrow \pi^*$ resonance. Finally, we described it by a theoretical calculation based on full-CI.

MO 27.8 Thu 16:15 P 204

Towards multi-color laser action spectroscopy of highly excited H_3^+ in the CSR — •L. Berger[1], J. Himmelsbach[1], M. Maxton[1], L. Enzmann[1], F. Grussie[1], L. Isberner[1], O. Novotný[1], V.C. Schmidt[1], D. Sharma[1,2], A. Znotins[1], and H. Kreckel[1] — [1]Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — [2]Department of Particle Physics and Astrophysics, Weizmann Institute of Science, Rehovot, Israel

The higher excitation spectrum above 16500 cm^{-1} of the simplest polyatomic molecule H_3^+ remains largely unexplored since these states are both experimentally and theoretically challenging to access. To bridge the gap to the measured but unassigned pre-dissociation spectrum above 35000 cm^{-1} [1] a multi-color action spectroscopy scheme has been proposed [2]. In the first step, the ions are pumped from the ground state to a metastable transition state above 10000 cm^{-1}, where the molecule begins to sample linear configurations. In a second step, these ions are excited to the regime of interest above 20000 cm^{-1} before they are dissociated with a UV laser and the dissociation products are recorded by a sensitive single particle detector. In this work we demonstrate the first step at the Cryogenic Storage Ring (CSR) in Heidelberg [3]. [1] Carrington et al., Acc. Chem. Res. 22, 218-222 (1989). [2] Znotins et al., J. Mol. Spectrosc. 378, 111476 (2021). [3] Maxton, Master Thesis (2025)

MO 28: Interaction with VUV and X-ray light I (joint session A/MO)

Time: Thursday 14:30–16:30 Location: N 2

Invited Talk MO 28.1 Thu 14:30 N 2

IR-laser induced dressing signatures in helium nanodroplets probed by coherent diffractive imaging — •Tom von Scheven, Björn Kruse, and Thomas Fennel — Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, D-18059 Rostock, Germany

Single-shot coherent diffractive imaging (CDI) enables the capture of a full diffraction image of a nanostructure using a single flash of XUV or X-ray light. The resulting scattering image encodes both the geometry and the optical properties of the target. So far, this method has mainly been employed for ultrafast structural characterization [1]. However, CDI can also be utilized to resolve ultrafast optical property changes caused by e.g. transient excitation from nonlinear scattering [2], or by illumination with a second ultra-short laser pulse.

Here, we explore the expected signatures for the latter case theoretically, where simultaneous exposure to a strong IR field can induce transient optical properties. To this end, the effective optical properties, emerging from the laser dressing, are extracted from the dipole response of a local quantum description based on an atom-like solution of the time-dependent Schrödinger equation. In a second step, we apply the well-known Mie-solution, to use the obtained optical properties in order to describe the resulting scattering process at helium nanodroplets and compare the results to recent experiments [3].

[1] I. Barke *et al.*, Nat. Commun. **6**, 6187 (2015)
[2] B. Kruse *et al.*, J. Phys.: Photonics **2**, 024007 (2020)
[3] J. Schäfer-Zimmermann *et al.*, arXiv, 2508.19936 (2025)

MO 28.2 Thu 15:00 N 2

Non-Hermitian X-Ray photonics and Exceptional Points in thin-film cavities with Mössbauer nuclei — •Fabian Richter[1], Lars Bocklage[2], Sven Velten[2], Ralf Röhlsberger[2], Xiangjin Kong[3], and Adriana Pálffy[1] — [1]Julius-Maximilians-Universität, Würzburg — [2]DESY, Hamburg — [3]Fudan University, Shanghai

Exceptional Points (EPs) mark non-Hermitian degeneracies where eigenvalues and eigenvectors coalesce, producing enhanced sensitivity to perturbations. While widely explored in optical gain-loss systems [1], translating the physics of EPs to the X-ray regime offers distinct advantages such as superior penetration depth, focusability, and detection efficiency.

Here, we investigate non-Hermitian X-ray photonics in thin-film cavities with ^{119}Sn Mössbauer nuclei under grazing-incidence illumination. In addition to theoretical modeling, we analyze experimental time spectra and reflectivity data recorded at PETRA III. The cavity geometry and incidence angle offer tunable control over dissipation [2], while a magnetic hyperfine field enables steering the system toward EPs. In theory, we identify the magnetic field strengths at which EPs emerge and predict qualitatively distinct features in the simulated time spectra. In the experimental time spectra, the situation is more complicated, especially as quadrupole splitting introduces additional spectral structure and increases the complexity of the eigenvalue problem, yet we are able to reliably extract the relevant signatures.

[1] L. Feng et al., Nature Photon. 11, 752-762 (2017).
[2] J. Evers, K. P. Heeg, Phys. Rev. A 88, 043828 (2013).

MO 28.3 Thu 15:15 N 2

Single-shot sorting of Mössbauer time-domain data at X-ray free electron lasers — •Miriam Gerharz and Jörg Evers for the Fe-57 EuXFEL-Collaboration — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Mössbauer spectroscopy is widely used to study structure and dynamics of matter with remarkably high energy resolution, provided by the narrow nuclear resonance line widths. However, the narrow width implies low count rates, such that experiments commonly average over extended measurement times or many x-ray pulses (“shots”). This averaging impedes the study of non-equilibrium phenomena. It has been suggested that X-ray free-electron lasers (XFELs) could enable Mössbauer single-shot measurements without averaging, and a proof-of-principle demonstration has been reported [1]. However, so far, only a tiny fraction of all shots resulted in signal-photon numbers which are sufficiently high for a single-shot analysis. In [2], we develop a sorting approach which allows us to include all data on a single-shot level, independent of the signal content of the individual shots. It utilizes the presence of different dynamics classes, i.e. different nuclear evolutions after each excitation. Each shot is assigned to one of the classes, which can then be analyzed separately. We envision that our approach opens up new grounds for Mössbauer science and beyond, enabling the study of out-of-equilibrium transient dynamics of the nuclei or their environment.

[1] Chumakov et al., Nature Phys 14, 261-264 (2018)
[2] Gerharz et al., arXiv:2509.15833

MO 28.4 Thu 15:30 N 2

Neural networks for diffraction image separation — •Nikita Morozov — European XFEL, Schenefeld, Germany

Newly available soft X-ray two-color FEL pulse mode at European XFEL opens a new path to the structural and plasma studies at the nanometer scale. The first pulse, designated as the pump, characterizes the initial state of the object, whereas the second probe pulse captures the system’s evolution following its interaction with the pump. The pulses are separated by a short time interval of less than 1 ps. Because this delay is shorter than the detector acquisition time, the state-of-the-art detectors are unable to capture two independent Coherent Diffractive Imaging (CDI) images corresponding to the pump and probe pulses. Instead, it records a single data frame that contains a superposition of CDIs from both FEL pulses, making it almost impossible to follow the evolution process.

This work presents machine learning-based solutions for separating the overlapping components in such data sets. We propose two methods: the first one is based on diffusion probabilistic models, a recent and powerful approach for image generation, and the second using feed-forward convolutional neural networks to solve the same task.

Ideally, after the image separation task is done, the pump and probe densities could be recovered using standard phase retrieval techniques, allowing the excitation-induced changes to be examined in a time-resolved manner.

MO 28.5 Thu 15:45 N 2

Laser-driven electron dynamics in helium nanodroplets retrieved from single-shot diffraction patterns — •B. Senfftleben[1,2,3], A. Colombo[1], A. Hoffmann[2], M. Sauppe[1,2], K. Kolatzki[1,2], B. Langbehn[4], J. Schäfer-Zimmermann[1,2], M. Kretschmar[2], M. Krause[2], T. Nagy[2], M. J. J. Vrakking[2], B. Schütte[2], and D. Rupp[1,2] — [1]ETH Zurich, Switzerland — [2]Max-Born-Institut Berlin, Germany — [3]European XFEL, Schenefeld, Germany — [4]TU Berlin, Germany

Coherent diffraction experiments on single particles using intense X-ray or XUV light sources have revolutionized the structural determination of fragile, short-lived nanoscale samples and their dynamics. However, electronic properties are also inherently encoded in the diffraction patterns, but their extraction requires new analysis methods. In our study, we employed a high-harmonic-generation (HHG) light source to perform NIR-XUV pump-probe experiments at photon energies near strong electronic resonances of helium droplets.

In this presentation, several of our analysis approaches to address challenges related to detection artifacts and the multicolor nature of HHG radiation will be discussed. Moreover, initial findings on ultrafast changes in the optical properties and, thus, on electron dynamics of helium nanodroplets will be presented.

MO 28.6 Thu 16:00 N 2

Fast Simulation of Wide-Angle Coherent Diffractive Imaging — •Paul Tuemmler, Julia Apportin, Thomas Fennel, and Christian Peltz — Institute of Physics, University of Rostock 18051, Rostock, Germany

Single-shot coherent diffractive imaging with intense XUV and soft X-ray pulses offers the exciting possibility of retrieving both the 3D structure and optical properties of nanoscale objects from a single diffraction pattern. Achieving this, however, requires an accurate description of the underlying wide-angle scattering and propagation effects, which are significantly more complex than in conventional X-ray diffraction.

In this talk, I will introduce the propagation multi-slice Fourier transform method (pMSFT) [1], a fast and accurate approach for simulating the scattering process in this regime. I will outline its derivation from first principles, introduce a unified physical picture to show its relation to existing methods, and finally present systematic benchmarks demonstrating its superior performance for wide-angle scattering.

[1] P. Tuemmler, et al., Laser Photonics Rev (2025): e02001 https://doi.org/10.1002/lpor.202502001

MO 28.7 Thu 16:15 N 2

K-edge core excitation and ionization of singly charged sulfur cations — •Simon Reinwardt[1], Patrick Cieslik[1], Ticia Buhr[2], Alexander Perry-Sassmannshausen[3], Stefan Schippers[3], Alfred Müller[3], Stephan Fritzsche[4,5], Florian Trinter[6], and Michael Martins[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [3]Justus-Liebig-Universität Gießen, Gießen, Germany — [4]Friedrich-Schiller-Universität Jena, Jena, Germany — [5]Helmholtz-Institut Jena, Jena, Germany — [6]Fritz-Haber-Institut, Berlin, Germany

Near-edge X-ray absorption spectroscopy on sulfur cations provides important reference data for X-ray telescopes and to investigate tender or soft X-ray induced fragmentation processes on sulfur-containing molecular ions. Using the photon-ion merged-beams technique, implemented at the Photon-Ion Spectrometer at PETRA III [1], we measured relative cross sections for twofold, threefold, fourfold, and fivefold photoionization of singly charged sulfur cations in the photon-energy range from 2460 eV to 2510 eV. To theoretically describe the relative cross sections of the different product charge states, we have calculated decay cascades with the Jena Atomic Calculator [2].

[1] S. Schippers *et al.*, J. Phys. B **47**, 115602 (2014).

[2] S. Fritzsche, Comput. Phys. Commun. **240**, 1 (2019).

MO 29: Cluster and Nanoparticles (joint session MO/A)

Time: Thursday 15:15–16:45 Location: P 105

Invited Talk MO 29.1 Thu 15:15 P 105

Charge and electronics in molecule activation by transition metal clusters — •Gereon Niedner-SChatteburg, Nils Wolfgramm, and Christoph van Wüllen — Fachbereich Chemie, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern

Isolated transition metal clusters (TMCs) serve as well established proxys for the characterization of elementary reaction steps and intermediates. The charge states of such clusters are subject of debate ever since. We have developed and applied a cryo trapping technique [1] that allowed us to characterize size selected TMCs and their adsorbates for their kinetic and spectroscopic properties [2-8]. Electronic characterization arose through novel X-ray techniques which we have brought to gas TMCs [9]. We have recently started a systematic quantum chemical survey of electronic effects along the N_2 activating reaction pathways of some selected clusters [10], and the conceptual findings of this survey shall be presented and discussed. [1] 10.1016/B978-0-12-814013-0.00019-3; [3] 10.1039/c5cp00047e; [2] 10.1021/acs.jpcc.6b12167; 10.1063/1.4997403 ; 10.1063/1.4997407; [5] 10.1007/s11244-017-0865-2 ; 10.1080/00268976.2021.1953172; [4] 10.1063/5.0064965 ; 10.1063/5.0064966; [5] 10.1063/5.0075289 ; 10.1063/5.0075286; [7] 10.1039/D0CP06208A ; 10.1063/5.0157218 ; 10.1063/5.0157217; [8] 10.1021/acs.jpclett.8b00093 ; submitted to Helv. Chim. Act. (2025); [9] 10.1103/PhysRevLett.107.233401 ; 10.1039/C5CP01923K ; 10.1063/1.4929482; [10] to be published

MO 29.2 Thu 15:45 P 105

Size characterization of doped rare-gas clusters utilizing rotational coherence spectroscopy — •Arne Morlok[1], Grzegorz Kowzan[2], Ulrich Bangert[1], Yilin Li[1], Frank Stienkemeier[1], and Lukas Bruder[1] — [1]University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg, Germany — [2]Nicolaus Copernicus University in Torun, Institute of Physics, Grudziadzka 5, 87-100 Torun, Poland

A prominent challenge in spectroscopy is to investigate individual molecules or their aggregates in a well-defined and controlled environment. This goal can be accomplished with cluster-isolation spectroscopy, a technique in which molecules are isolated in or on the surface of rare-gas clusters. A complication of this technique is that the clusters, which are produced in a supersonic expansion, do not have a uniform size but follow a broad size distribution dependent on the expansion conditions. Although semi-empirical scaling laws based on the expansion parameters have been derived in order to predict the mean cluster size, results seem to underestimate the actual cluster size in comparison with experimentally determined size distributions. In this contribution, a novel spectroscopic approach is discussed to determine the mean cluster size of neutral rare-gas clusters. The technique is based on already known methods from rotational coherence spectroscopy. Results suggest a new scaling regime for the mean cluster size in the already established model in a certain parameter range.

MO 29.3 Thu 16:00 P 105

Measuring the speed of interatomic Coulombic decay in helium nanodroplets — •Asbjørn Ørnemark Laegdsmand[1], Ltaief Ben Ltaief[2], Eva Klimesova[3], Keshav Sishodia[3], Martin Albrecht[3], and Marcel Mudrich[1] — [1]Institute of Physics, University of Kassel, 34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [3]ELI Beamlines, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 252 41 Dolní Břežany, Czech Republic

Helium nanodroplets are an interesting *test tube* for many types of interatomic reactions. In this work we have looked at both interatomic Coulombic decay (ICD) and laser-assisted electron scattering (LAES). We have measured the rate of ICD in lithium-doped helium nanodroplets by an EUV-pump NIR-probe scheme.

The nanodroplets are resonantly excited into the 1s 2p ^{1}P state with a 21.6 eV pump pulse and multi-photon ionized with an 1.56 eV probe pulse. ICD and LAES electrons are detected with in a magnetic bottle electron spectrometer. Arrival of the probe pulse ionizes most of the 1s 2p ^{1}P He, quenching the ICD process. Thus by varying the time delay between pump and probe we measure the speed of the ICD for different droplet sizes.

From the resulting electron spectra we distinguish several ionization pathways, such as ICD, LAES and above threshold ionization. We model the dynamics of the different pathways by rate equations and estimate their contribution to the total electron yield as a function of pump-probe delay time.

MO 29.4 Thu 16:15 P 105

An optical laser blade setup for the detection of isolated nanoparticles — •Constantin Koch[1], José Gómez Torres[1], David Biner[1], Indrani Dey[1], Frederic Ussling[1], Linos Hecht[1], Yves Acremann[1], Isabelle Bollier[1], Alessandro Colombo[1], Ehsan Hassanpour[1], Katharina Kolatzki[1], Changji Pan[1], Mario Sauppe[1], Lea Schüpke[1], Björn Senfftleben[1], Hanchao Tang[2], Arnab Choudhury[2], Bruce Yoder[2], Ruth Signorell[2], and Daniela Rupp[1] — [1]D-PHYS, ETH Zurich — [2]D-CHAB, ETH Zurich

Coherent diffraction imaging (CDI) of free-flying water nanodroplets with our high-intensity extreme ultraviolet (XUV) beamline requires optimal overlap of droplet beam and micrometer-sized XUV focus. So far, this was difficult to achieve because of the small hitrates and large variability of the single-shot signals from XUV diffraction. We present the design, setup and comissioning of an optical laser blade, that makes nanoparticles in the interaction region directly visible and enables a quantitative characterization of the water source. A continuous-wave 450 nm laser is shaped into a thin horizontal laser sheet crossing the droplet beam. The scattered light is recorded with a CMOS camera adapted for vacuum compatibility. We observe clear signal from single droplets in the few hundred nm range and achieved a fast and reliable alignment procedure. The consistent signal also allowed us identify previously overlooked problems in the injector system and to obtain a three-dimensional density distribution of the droplet beam in our vacuum chamber.

MO 29.5 Thu 16:30 P 105

Uptake of Ammonia onto Mixed Sodium Sulfate/Bisulfate Cluster Ions Studied in a Cryogenic Ion Trap — •Kevin Li, Yihui Yan, and Jozef Lengyel — School of Natural Sciences, Technical University of Munich, Garching, Germany

Understanding the earliest stages of atmospheric new particle formation (NPF) requires direct measurements on sub-nanometer molecular clusters, yet such studies remain experimentally challenging. To investigate this size range, we have developed a cryogenic ion trap mass spectrometer for kinetic studies with mass-selected cluster ions under multicollisional conditions. The instrument utilizes a ring-electrode ion trap, which enables stable confinement and allows for long reaction times of up to seconds. Therefore, the trap provides a powerful platform for investigating reaction pathways relevant to atmospheric aerosol formation.

In this study, we characterize the performance of the cryogenic ion trap and show its capabilities in a model study measuring uptake of gaseous ammonia onto mixed sodium sulfate and bisulfate ions. We further highlight that investigating mixed multicomponent clusters can reveal synergistic effects in NPF, where different components jointly enhance the uptake efficiency. In mixed sodium sulfate-bisulfate clusters, bisulfate units govern the number of uptaken ammonia molecules, whereas sulfate units control the reaction rate. With these experiments, we demonstrate the instrument's ability to investigate reaction pathways relevant to NPF.

MO 30: Poster – Molecular Spectroscopy

Time: Thursday 17:00–19:00 Location: Philo 1. OG

MO 30.1 Thu 17:00 Philo 1. OG

Empowering Research with Time-Resolved Fluorescence Methods: A KeyLab Approach — •Lisa Günther[1,2,3] and Jürgen Köhler[1,2,3] — [1]Spectroscopy of soft Matter, University of Bayreuth — [2]Bayreuth Institute for Macromolecular Research (BIMF), University of Bayreuth — [3]Bavarian Polymer Institute, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Addressing today's complex scientific questions requires interdisciplinary approaches that integrate advanced analytical techniques with a broad range of sample systems. However, researchers often face limitations due to restricted access to specialized instrumentation or the expertise needed to design, perform, and interpret experiments. Shared laboratories and core facilities help overcome these barriers by providing advanced infrastructure, methodological know-how, and collaborative environments. The KeyLab Optical Spectroscopy at the Bavarian Polymer Institute connects method development with user-oriented applications by combining commercial and custom-built experimental platforms within a flexible framework. A commercial system offers advanced fluorescence lifetime, correlation, and single-molecule capabilities, while a complementary custom-built setup adds modular design and cryogenic capability for tailored studies under variable conditions. From polymer aggregates and perovskite nanostructures to biological photophysical systems, the KeyLab provides a versatile environment for exploring complex photophysical phenomena across disciplines.

MO 30.2 Thu 17:00 Philo 1. OG

High-Resolution Excitation Spectroscopy of Acridine Derivatives and their Complexes with Water — •Kaleb Strahringer, Aleksandr Demianenko, Frank Stienkemeier, and Sebastian Hartweg — Universität Freiburg, Phys. Institut, 79104 Freiburg

Using sunlight to split water into oxygen and hydrogen offers a sustainable route to producing hydrogen as a source of energy from abundant resources. While directly breaking the H-O bond requires 6.66 eV, excitation of a chromophore that mediates the reaction via electron-driven proton transfer (EDPT) reactions, can significantly reduce the necessary photon energy. Potential chromophores include aromatic N-heterocycles that have been studied experimentally [1] and theoretically [2]. Larger polycyclic chromophores are predicted to require lower excitation energies to enable EDPT reactions. For this reason, and as a prerequisite for future time-resolved studies, we plan to investigate promising acridine derivatives and their complexes with water with high-resolution excitation spectroscopy. In our setup, we use helium nanodroplet isolation spectroscopy to efficiently cool isolated chromophore molecules and form their complexes with water under controlled conditions. Using high-resolution nanosecond-laser fluorescence spectroscopy and resonance-enhanced multiphoton ionization (REMPI) schemes to probe dark states, we aim to obtain detailed insights into the chromophores' vibronic structure and relaxation pathways, and how they are affected by the presence of water.

[1] Esteves-López et al., Phys. Chem. Chem. Phys. 18 (2016) 25637

[2] Liu et al., Chem. Phys. 464 (2016) 78

MO 30.3 Thu 17:00 Philo 1. OG

Experimental setup for recurrent fluorescence studies of cold trapped molecular ions — •Nariste Asanova, Surabhi Gupta, Suvasis Swain, Henrik Haak, Gerard Meijer, and Jascha A. Lau — Fritz-Haber-Institute der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Emission lines in the visible and infrared range detected in interstellar environments are frequently attributed to carbon-rich species, such as polycyclic aromatic hydrocarbons (PAHs) and linear carbon chains. Therefore, it is important to study the radiative cooling process of these molecular systems. We are developing a new experimental setup that employs a linear Paul trap, in which a sufficiently dense, cold ion cloud is trapped at the interaction center to allow for dispersed fluorescence spectroscopy in millisecond timescale. The main focus is on recurrent fluorescence, which has been recently experimentally proven. The ion optics of the ion source, mass spectrometer, and the ion trap were optimized in SIMION 8.2 to ensure efficient loading of the trap. Once the ions are inside the trap, a short pulse of cold (4 K) He/H2 buffer gas is released, resulting in internal and translational cooling of the ions through collisions. The gas pressure must decay on a short timescale (˜10 ms) to prevent quenching of the fluorescence signal. Time-dependent pressure curves for each stage were modeled using Molflow+ to optimize gas conductance out of the trap while minimizing stray light. The signal is measured by a monochromator, with time-resolved single-photon counting using a photomultiplier tube and dispersed spectra recorded by an iCCD camera.

MO 30.4 Thu 17:00 Philo 1. OG

Intermolecular vibrational wavefunctions of OH$^+$He — •Nima-Noah Nahvi and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

To study the weak interaction of helium with open-shell cations, it is important to precisely determine the zero-point energy and other vibrational effects. Here, we present calculations of the multidimensional intermolecular vibrational wavefunction of the OH$^+$He dimer. Our approach consists of coupled cluster calculations along all degrees of freedom, fitting and correcting the resulting potential energy surfaces and numerically evaluating the Schrödinger equation. The calculations include both the ground and first excited state of the system, allowing the simulation of the electronic spectrum. Furthermore, we analyze the vibrational dynamics of OH$^+$He in its excited state by time-propagating the calculated wavefunctions. Our results can be used to interpret the optical action spectrum of the first excited state of OH$^+$He, which was obtained through UV induced photodissociation inside a cryogenic ion trap.

MO 30.5 Thu 17:00 Philo 1. OG

Photoelectron Spectroscopy of Thiaadamantane — •Domenik Schleier, Parker Crandall, Simone Stahl, Sebastian Voelz, and Otto Dopfer — Institut für Physik und Astronomie, TU Berlin, Germany

Diamondoids are three dimensional organic molecules that are derived from the diamond lattice structure. As such, they contain no aromatic system, rendering their electronic structure distinctly different from polycylic aromatic hydrocarbons. Nonetheless, they exhibit broadly tunable optical properties as well as a high chemical and thermal stability, making them suitable for applications in photonics, material science and medicine. The proliferation of nanodiamonds in extraterrestrial environments suggests that their molecular derivatives play important roles in astronomy as well. To evaluate their presence, their electronic structure and photostability need to be characterized. While regular diamondoids exhibit broad and featureless optical spectra due to ultrafast non-radiative deactivation, heteroatom substitutions of the cage-carbon atoms increases their excited state lifetime and possibly their photostability. To further study the effect of heterosubstitution on the electronic structure of diamondoids we study the electronic structure of Thiaadamantane (ThiaAda) by photoelectron spectroscopy and its photodecomposition via quantum chemistry. We find an abiabatic ionization energy of 8.04 eV for ThiaAda and characterize multiple excited states.

MO 30.6 Thu 17:00 Philo 1. OG

Competition Between NH...π Hydrogen Bonding and Charge Resonance Interactions in Aromatic Heterodimer Radical Cations Revealed by IR spectroscopy — •Dashjargal Arildii and Otto Dopfer — Technische Universität Berlin, Berlin, Germany

In aromatic radical cation dimers, charge resonance (CR), in which a positive charge is delocalized over both monomers, is one of the strongest forces with binding energies of $\sim$100 kJ/mol, favoring sandwich structures. The strength of CR depends strongly on the differences between the ionization energies (ΔIE) of the interacting monomers. Thus, homodimers such as the pyrrole dimer cation (Py$_2{}^+$) have the strongest CR. However, in heterodimers, CR is weakened, allowing other bonding motifs, such as NH$\cdots\pi$ H-bonding to compete, favoring T-shaped structures. Herein, we investigate the binding motifs of pyrrole$^+$-benzene (Py$^+$Bz), pyrrole$^+$-toluene (Py$^+$Tol), and pyrrole$^+$-naphthalene (Py$^+$Np) heterodimers, with ΔIE=1.03, 0.59, and -0.06 eV, respectively, using infrared photodissociation spectroscopy (IRPD) and density functional theory calculations. Analysis of IRPD spectra of mass-selected Py$^+$Bz, Py$^+$Tol, and Py$^+$Np, combined with geometric parameters of intermolecular structures, reveals that competition between NH$\cdots\pi$ H-bonding and CR interaction with respect to ΔIE of the monomers.

MO 30.7 Thu 17:00 Philo 1. OG

Implementing a multi-color laser action spectroscopy setup to measure highly excited states of H_3^+ ions in the CSR — •J. Himmelsbach[1], L. Berger[1], M. Maxton[1], L. Enzmann[1], F. Grussie[1], L. Isberner[1], O. Novotný[1], V. C. Schmidt[1], D. Sharma[1,2], A. Znotins[1], and H. Kreckel[1] — [1]Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — [2]Department of Particle Physics and Astrophysics, Weizmann Institute of Science, Rehovot, Israel

H_3^+ is one of the main drivers for astrochemistry in diffuse interstellar clouds and serves as a benchmark for theory as the simplest polyatomic molecule. Despite being extensively studied in the past, its highly excited states above 16 500 cm^{-1} remain largely unexplored, as they are both experimentally and theoretically challenging to access. A multi-color action spectroscopy scheme has been proposed to measure states above 20 000 cm^{-1} [1], providing a bridge to the unassigned pre-dissociation spectrum around 35 000 cm^{-1} [2]. In this approach, cold molecules stored in the Cryogenic Storage Ring (CSR) are excited in two steps from their ground state into the region of interest via a long-lived metastable state. The molecule is then dissociated with a UV laser to measure the fragments using a single particle detector. Recently, the first excitation step has been successfully demonstrated [3]. This poster focuses on the experimental realization of the second excitation step and the final dissociation step. [1] Carrington et al., Acc. Chem. Res. 22, 218-222 (1989). [2] Znotins et al., J. Mol. Spectrosc. 378, 111476 (2021). [3] Maxton, Master Thesis (2025)

MO 30.8 Thu 17:00 Philo 1. OG

Probing Electronic-Nuclear Coupling with MIR-XUV Spectroscopy — •Pankaj Seliya, Lina Hedewig, Carlo Kleine, Christian Ott, and Thomas Pfeifer — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

The interplay between vibrational and electronic motions governs various molecular phenomena including energy dissipation, delocalization, and charge transfer [1]. Existing methods to study electronic-nuclear coupling, such as impulsive Raman [2] and two-dimensional vibrational-electronic (2DVE)/electronic-vibrational (2DEV) [3] spectroscopy provide selectivity only either along vibrational or electronic coordinates, but not both. Impulsive Raman with XUV/soft-X-ray probe provides electronic selectivity, but broadband near-IR/UV-Vis excitation drives multiple vibrational modes [2]. In contrast, 2DVE offer vibrational selectivity via resonant mid-IR(MIR) excitation, but visible probes lack electronic specificity. Here, we introduce an approach that accesses vibronic coupling with both vibrational and electronic selectivity, using resonant MIR pulses for mode-specific vibrational excitation and XUV pulses for element-specific probing of electronic dynamics. We test our setup with helium atoms, observing light-induced states [4] generated by exciting the 1sns /1snd states via one-photon XUV absorption together with absorption/emission of a one MIR photon. Experiments are currently being extended to molecules such as SF6 and N2O. References: [1] Struct. Dyn. 4, 061508 (2017) [2] J. Chem. Phys. 156, 114304 (2022) [3] J. Chem. Phys. 147, 094202 (2017) [4] Physical Review A 86, 063408 (2012)

MO 30.9 Thu 17:00 Philo 1. OG

Vibrationally resolved core excitation of the CN$^+$ molecular ion — •Maria Tatsch[1], Anastasia Andreeva[2], B. Michel Döhring[1,3], Pierre-Michel Hillenbrand[4], Micheal Martins[2], Alfred Müller[1], Simon Reinwardt[2], Jörn Seltmann[5], Julius Schwarz[2], Florian Trinter[6], and Stefan Schippers[1,3] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen — [2]Institut für Experimentalphysik, Universität Hamburg — [3]Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt — [4]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt — [5]Deutsches Elektronen-Synchrotron DESY, Hamburg — [6]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Near-edge x-ray absorption fine structure spectroscopy (NEXAFS) is a powerful tool to probe electronic core excitations. At the PETRA III synchrotron facility (DESY, Hamburg) operating at the soft-x-ray beamline P04, the PIPE setup enables photon-ion merged beams experiments. The brilliant PETRA III synchrotron light enables vibrationally resolved core-excitation spectroscopy and provides access to high resolution measurements. Core-excited molecular ions pose several new challenges, such as unpaired valence electrons and core-valence correlation effects. Our results provide the community with valuable benchmark data to guide the development of accurate theoretical descriptions of core-excited diatomic molecules. We present the current status of our data analysis on x-ray absorption studies of CN$^+$ molecular ion.

MO 30.10 Thu 17:00 Philo 1. OG

Design for a monochromatic, high-repetition-rate XUV beamline for time-resolved photoelectron-photoion coincidence spectroscopy — •Merline Cherukarathadathil Ulahannan, Ulrich Bangert, and Sebastian Hartweg — Institute of Physics, University of Freiburg, Freiburg, Germany

We present our plans for a monochromatic XUV beamline with high-repetition rates of up to 120 kHz for time-resolved photoelectron photoion coincidence spectroscopy. The beamline will be based on a cascaded harmonic generation scheme [1] driven by an Yb Laser. The 800 μJ near IR pulses will be first spectrally broadened by self-phase modulation in a gas-filled multipass cell and compressed to ~40 fs before the second and third harmonic of the 1030 nm fundamental are generated in a set of BBO crystals. The resulting visible and ultraviolet laser pulses will be used to efficiently drive the HHG process in a gas jet producing XUV radiation in the range between 12 and 20 eV. After separation of the XUV from the driving field we will use a time-preserving monochromator [2] with a single plane diffraction grating in off-plane geometry for spectral selection while maintaining pulse durations of tens of femtoseconds. A home-built nonlinear optical parametric amplifier pumped by the same Yb Laser will supply frequency-tunable ultrashort pump pulses in the visible and UV spectral range. This beamline will be used in performing time-resolved XUV photoelectron-photoion coincidence spectroscopy in molecular complexes. Reference:1.Comby et al., Opt. Express 27, 20383 (2019). 2.Frassetto et al., Opt. Express 19, 19169 (2011).

MO 30.11 Thu 17:00 Philo 1. OG

Development of an ns-OPO/OPA Mid-Infrared Source for Molecule Detection by THG Spectroscopy — •Noah Dornhecker and Thomas Halfmann — TU Darmstadt Institut für Angewandte Physik, Darmstadt, Germany

We report on progress towards a nanosecond mid-infrared laser source based on a compact, all-solid-state OPO-OPA architecture, developed to provide narrowband, tunable mid-infrared (MIR) pulses and pulse energies at the mJ level, e.g., for nonlinear spectroscopy of molecular samples. In particular, we aim at a wavelength of 4.3 μm for the detection of CO_2 via resonantly enhanced THG spectroscopy. The system employs an injection-seeded, frequency-doubled Nd:YAG pump at 532 nm to drive an OPO stage, generating a signal wave at 853 nm and an idler wave at 1412 nm. The latter seeds an OPA stage, pumped by the fundamental wave at 1064 nm of the Nd:YAG laser, allowing efficient difference-frequency generation towards the MIR. Initial results demonstrate stable operation of the OPO stage with idler pulse energies above 190 μJ, distinctly narrowed spectra under injection seeding, and spatial beam profiles close to Gaussian. As first results from the OPA stage, we meanwhile achieved output pulse energies of 13 μJ at a wavelength of 4.3 μm, which are subject now to further improvement. From simulations, we confirmed that with a seed pulse energy of 190 μJ, we can reach the mJ regime from the OPA stage. These characteristics provide a robust seed for high-gain MIR amplification targeting mJ-level pulse energies. We demonstrate the applicability of the system for molecule detection via nonlinear spectroscopy.

MO 30.12 Thu 17:00 Philo 1. OG

Broadband UV/Vis sub-20 fs transient absorption spectroscopy — •Marvin Krupp and Stefan Lochbrunner — Institute of Physics, Rostock, Germany

Studies on ultrafast chemical reaction steps, such as proton transfer, call for broadband spectroscopy with a time resolution below typical vibrational periods. In this work, a noncollinear optical parametric amplifier (NOPA) pumped by a Ti:Sa laser system is optimized for sub-20 fs pulses with a particular broad spectrum thus they are suitable as probe pulses for broadband transient absorption spectroscopy. The broadband NOPA enables spectral detection ranges of 490 to 900 nm and after frequency doubling of about 300 to 420 nm. Using chirped mirrors for compression, we can decrease the signal rise time at time zero of the experiment down to less than 20 fs across most spectral components. We compare these broadband NOPA measurements with uncompressed white light probing. First measurements on 2-(2*-hydroxyphenyl)-benzothiazole (HPBT) have been performed, in which proton transfer is estimated to happen on a timescale of 30-40 fs. In agreement with previous studies [1], we confirm their observations and provide a broadband analysis of the underlying proton-transfer dynamics. [1] J. Phys. Chem. A 2003, 107, 49, 10580*10590

MO 30.13 Thu 17:00 Philo 1. OG

Measuring a complete quantitative photon-excitation photon-emission map of molecular hydrogen — •Adrian Krone, Johannes Viehmann, Dana Bloss, Niklas Golchert, Emilia Heikura, Catmarna Küstner-Wetekam, Lutz Marder, Yusaku Terao, Andreas Hans, and Arno Ehresmann — Institute of Physics and CINSat, University of Kassel, 34132 Kassel, Germany

Fluorescence spectra of molecular hydrogen singly-excited by narrow bandwidth ($\approx 1\,\mathrm{meV}$) synchrotron radiation are measured in 1 meV steps scanning over all rovibronic excitations of room-temperature H_2. The spectra are combined to construct a quantitative photon-excitation photon-emission (PhexPhem) map, which can provide improved insights into astronomical data from UV telescopes. A prominent feature of the H_2 PhexPhem map are the Condon diffration bands, which can be used to extend benchmarking of potential energy curves to be sensitive to their shape at large internuclear distances.

MO 30.14 Thu 17:00 Philo 1. OG

Towards infrared spectroscopy of molecular ions in an electrostatic ion beam trap — •Antonia Schaffert[1], Deepak Sharma[1,2], Klaus Blaum[1], Oded Heber[2], Thomas Henning[3], Stav Knaffo[2], Sunil Kumar[4], Michael Rappaport[2], Andreas Wolf[1], Daniel Zajfman[2], and Holger Kreckel[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg — [2]Weizmann Institute of Science, Rehovot, Israel — [3]Max-Planck-Institut für Astronomie, Heidelberg — [4]IISER Tirupati, India

The chemistry of complex organic molecules in interstellar space is at the forefront of molecular astrophysics [1]; however, laboratory spectroscopy with complex species is rather challenging. For complex molecular ions, in particular, no established technique exists for gas phase spectroscopy. We are developing an experimental setup to perform infrared spectroscopy of stored molecular ions using an electrostatic ion beam trap (EIBT) [2]. The molecular ions are injected into the EIBT and reflected between two electrostatic mirrors. A characterization of the beamline and first results of the dynamics of trapped ions using a room-temperature EIBT are presented in this poster. For future spectroscopy measurements a cryogenic EIBT will be installed and combined with a sensitive mid-infrared photon detector.

[1] Herbst E, Vidali G, Ceccarelli C, ACS Earth Space Chem. 4, 488 (2020)

[2] D. Zajfman et al., Phys. Rev. A 55, R1577 (1997)

MO 30.15 Thu 17:00 Philo 1. OG

Shedding Light on $(\mathrm{SiC})^+_{1,2}$: First Laboratory Spectra Obtained by Electronic Photodissociation — •Kai Pollow, Alexander Breier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

Silicon carbide ions ($\mathrm{Si_nC_m^+}$) are expected in carbon-rich circumstellar environments such as those around asymptotic giant branch stars[1,2]. Several small neutral $\mathrm{Si_nC_m}$ species are known in the interstellar medium[3], but their cations remain unidentified due to missing spectroscopic data[4]. Spectra of $\mathrm{Si_nC_m^+}$ are therefore essential for assessing their role in ion–molecule chemistry and silicon carbide dust formation.

We present the first laboratory spectra of $(\mathrm{SiC})^+_{1,2}$, recorded via vibronic photodissociation of mass-selected ions in a quadrupole/time-of-flight tandem mass spectrometer with a laser vaporization source[4]. The spectra exhibit clear vibrational structure, and the derived parameters agree with quantum-chemical predictions.

References:

[1] T. Chen et al., *Mon. Not. R. Astron. Soc.* **509**, 5231 (2022).

[2] M. C. McCarthy et al., *J. Mol. Spectrosc.* **356**, 7 (2019).

[3] S. Massalkhi et al., *Astron. Astrophys.* **611**, A29 (2018).

[4] M. Förstel et al., *J. Mol. Spectrosc.* **377**, 111427 (2021).

MO 30.16 Thu 17:00 Philo 1. OG

From Gas-phase to liquid phase: probing the electronic structure of amino acids with X-ray spectroscopy — •Juliette Leroux[1,2], Nicolas Velasquez[3], Jean-Yves Chesnel[2], Markus Ilchen[1], and Sadia Bari[4] — [1]Universität Hamburg, Hamburg, Germany — [2]CIMAP, Caen, France — [3]Fritz-Haber Institut, Berlin, Germany — [4]Deutsches Elektronen Synchrotron, Hamburg, germany

The isolation of biomolecules in the gas phase eliminates all interactions with the solvent, allowing for stepwise control of these interactions by progressively increasing the number of bound water molecules, thereby bridging the gap between isolated molecules and aqueous conditions. Over the past three decades, experimental techniques have been developed to study hydrated species in the gas phase. Comparing the gas-phase structure with that of singly hydrated complexes provides insight into the influence of a single water molecule on molecular properties. In contrast, liquid-phase studies allow us to probe the influence of water as a bulk solvent and to approach conditions relevant to biology. X-ray radiation provides a local probe of the atomic environment through electronic excitations of core electrons to unoccupied molecular orbitals, thereby capturing both the electronic and geometric structure of the system under investigation. In this study, we combine X-ray absorption spectroscopy with tandem mass spectrometry to obtain information on the electronic structure of singly hydrated, protonated phosphotyrosine. We further explore the influence of the solvent on phosphotyrosine using liquid-jet photoelectron spectroscopy spanning the soft to tender X-ray domain.

MO 30.17 Thu 17:00 Philo 1. OG

Simulations of the dissociation of $\mathbf{CH^+, NH^+}$, and $\mathbf{OH^+}$ — •Filipp Junker[1], Simon Reinwardt[1], Anastasia Andreeva[1], Pierre-Michel Hillenbrand[2], Jörn Seltmann[3], Julius Schwarz[1], Ticia Buhr[3], Alexander Perry-Sassmannhausen[4], Alfred Müller[4], Stefan Schippers[4,5], Florian Trinter[6], and Michael Martins[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]I. Physikalisches Institut, Justus-Liebig-Universität, Gießen — [5]Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt — [6]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Molecular ions are able to heavily influence chemical reactions due to their high reactivity, thus it is crucial to learn about their electronic properties in order to understand the reaction dynamics. In a first step to achieve this, the objective is to investigate several ionic molecular systems, namely CH^+, NH^+, and OH^+, by performing multi-configurational self-consistent field (MCSCF) calculations. The kinetic energy release (KER) of the dissociating molecules is calculated by classical propagation on the potential energy curves for the various core-excited states and a Monte-Carlo simulation of the Auger-Meitner decay in order to gain insights about the ultrafast dissociation dynamics. This has been shown in a previous work for HF^+ as a model system. These results will be compared to experimental data recorded at Photon-Ion endstation at PETRA III (PIPE).

MO 30.18 Thu 17:00 Philo 1. OG

The magnetic hyperfine structure of 1-indanol — •Kilian Hügel[1,2], JuHyeon Lee[1], Shilpa Yadav[1], Sejun An[1], Boris G. Sartakov[1], Gerard Meijer[1], and Sandra Eibenberger-Arias[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin 14195, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany

Hyperfine interactions in molecules lead to small splittings of the energy levels due to various coupling mechanisms [1]. Studying such interactions is useful for example in the investigation of molecular geometries and for the design of quantum control experiments.

In our group, we are interested in the hyperfine structure of 1-indanol since it is the target molecule in our enantiomer-specific state transfer (ESST) experiments enabling quantum control of chiral molecules [2,3]. To investigate the hyperfine structure of such a complicated molecule with ten nuclear spins, we performed UV-microwave double-resonance spectroscopy in a cold, seeded molecular beam. Additionally, we developed a theoretical model treating the nuclear spin-spin interactions leading to 672 hyperfine lines per rotational transition connected to the absolute ground state. The calculated spectra match the measurements closely, confirming the theoretical model and enabling predictions of hyperfine effects in 1-indanol.

[1] C. H. Townes and A. L. Schawlow. Microwave Spectroscopy (Dover Publications, Mineola, New York, 1975). [2] A. O. Hernandez-Castillo et al. Phys. Chem. Chem. Phys. 23, 7048-7056 (2021). [3] JH. Lee et al. Nat. Commun. 15, 7441 (2024).

MO 30.19 Thu 17:00 Philo 1. OG

Electronic Spectra of Doped Diamondoid Cations — •Parker Crandall, Ronja Schramm, Sebastian Völz, Domenik Schleier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Berlin, Germany

We present our recently measured gas-phase photoelectron spectra (PES) of doped (cage-modified) diamondoids, namely 2-oxaadamantane, 2-thiaadamantane, and urotropine, to investigate the excited electronic states of their respective cations. These are interpreted with the aid of quantum chemical calculations and compared to the PES spectra of previously measured diamondoids. Heteroatom substitution within the carbon-cage network yields large band gaps between the ground and first excited states. Furthermore, vibronic fine structure is observed in the higher energy bands that is not observed in the spectra of the bare and functionalized diamondoids. Electronic photodissociation (EPD) spectroscopy reveals that in the case of urotropine$^+$, resolved vibronic structure attributed to the $D_3(^2A_1) \leftarrow D_0(^2A_1)$ electronic transition appears at a band origin of 29,990 cm^{-1} (333.4 nm) and grows increasingly more congested toward higher photon energy, suggesting considerable geometric distortion upon electronic excitation of the Jahn-Teller distorted ground electronic state. These measurements provide critical reference data for astronomical searches in the pursuit of a broader understanding of the chemical inventory of the interstellar medium.

MO 30.20 Thu 17:00 Philo 1. OG

Velocity Map Imaging Spectrometer Optimized for Reduction of Background Electrons from Scattered UV Light — •Fabian Westmeier, Nicolas Ladda, Jochen Mikosch, and Arne Senftleben — Institute of Physics, University of Kassel, Germany

Velocity map imaging spectroscopy is a powerful technique for detecting the momentum distribution of photoelectrons resulting from the ionization of atoms, molecules, clusters, or surfaces. However, when used with ultraviolet light sources, scattered photons can lead to the emission of photoelectrons from the spectrometer's electrodes, giving rise to severe noise superimposing the desired signal. We present a velocity map imaging spectrometer optimized to reduce such unwanted background signals. The primary modifications to the conventional design include spectrometer electrode geometries with small cross sections exposed to the scattered photons, blocked pathways for photoelectrons from the electrodes to the detector, and the incorporation of optical baffles to confine the solid angle of scattered light. Compared to a conventional design optimized solely on the spectrometer's photoelectron momentum resolution, we have achieved the elimination of 99.9% of the background noise without noticeably compromising the resolution. Note that most of the improvements were achieved without the necessity of high-grade windows, reducing the sensitivity to window degradation by UV light. We give general guidelines on efficiently coping with the long-standing experimental problem of electron background originating from scattered light by considering it already in the design stage of a new spectrometer.

MO 30.21 Thu 17:00 Philo 1. OG

Exploring Relaxation Mechanisms of Inner-shell Ionized Iodide Anions in Water — •Yusaku Terao, Dana Bloss, Gabriel Klassen, Johannes Viehmann, Adrian Krone, Niklas Golchert, Arno Ehresmann, and Andreas Hans — Universität Kassel, Institut für Physik und CINSaT, Heinrich-Plett-Strße 40, 34132 Kassel

Radiation effects in matter in aqueous environments are of great interest because many aspects remain poorly understood, although improved knowledge is essential for radiation protection and therapy. Understanding relaxation processes following excitation or ionization in biologically relevant systems requires considering interactions between solutes and surrounding water. The advent of liquid microjet techniques has enabled synchrotron-based studies of various liquid-phase phenomena. In particular, the discovery of interatomic and intermolecular decay processes, which dissipate energy and charge to neighboring species, has shown that solvation shells actively participate in post-ionization relaxation. Although these processes generally occur with lower probability than Auger decay, their identification has significantly revised the conventional picture. To the best of our knowledge, such interatomic/intermolecular decay has so far been demonstrated only for cations and dications in aqueous solution, with no clear evidence for anions. Here, we investigate iodide anions following inner-shell (3d, 4d) ionization to obtain fingerprints of possible interatomic/intermolecular decay channels and competing Auger cascades. The results were obtained using synchrotron radiation, a liquid microjet, and multielectron coincidence spectroscopy.

MO 30.22 Thu 17:00 Philo 1. OG

Wave packet interferometry with single LH2 complexes at ultrafast timescales — •Paul Recknagel[1], Stephan Wiesneth[1], Richard Hildner[2], Richard J. Cogdell[3], Alastair T. Gardiner[4], and Jürgen Köhler[1] — [1]Spectroscopy of soft Matter, University of Bayreuth, 95440 Bayreuth, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [3]School of Molecular Biosciences, Glasgow University, UK — [4]Institute of Microbiology of the Czech Academy of Sciences Třeboň, Czech Republic

Photosynthesis relies on capturing light energy by chromophores that are embedded in a network of pigment-protein complexes. The efficiency of this process depends crucially on the fine tuning of the electronic properties of the chromophores and their couplings to the protein environment. However, such complexes are flexible structures, that introduces a microscopic randomness which affects the delicate coordination of the mutual interaction strengths between chromophores and the protein scaffold. The peripheral light-harvesting complex LH2 from purple bacteria is one of the most studied model systems for understanding photosynthesis on a molecular level. We combined ultrafast time-resolved spectroscopy and linear fluorescence excitation spectroscopy to elucidate the energy transfer pathways (and the fluctuations thereof) within single LH2 complexes[1]. [1] S.Wiesneth et al, J. Am. Chem. Soc. 2025, 147, 40537-40546 (2025)

MO 31: Poster – Collisions, Scattering and Correlation Phenomena (joint session A/MO)

Time: Thursday 17:00–19:00 Location: Philo 1. OG

MO 31.1 Thu 17:00 Philo 1. OG

Relativistic S-Matrix Calculations of Compton Scattering from Bound Electrons — •Nick Marius Mayer[1,2], Jonas Sommerfeldt[3], and Andrey Surzhykov[1,2] — [1]Technische Universität, Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt. Braunschweig, Germany — [3]Laboratoire Kastler Brossel, Paris, France

Compton scattering is a fundamental process in which an incoming photon is inelastically scattered by an electron bound to an atomic nucleus. It finds important applications across many areas of modern science, ranging from medical radiotherapy to X-ray polarimetry. With regard to the latter, we present theoretical analyses of Compton scattering by bound electrons, with special focus on polarization effects. In particular, we discuss calculations based on S-matrix theory. To carry out these calculations, we developed a program that numerically solves the radial Dirac equation accurately for a bound electron in the central nuclear potential, approximated here by a Coulomb potential. Based on this approach, detailed calculations of the doubly differential cross section (DDCS) and the polarization properties of photons scattered by K-shell electrons can be carried out across a broad range of energies and for arbitrary polarization states of the incident photon beam.

MO 31.2 Thu 17:00 Philo 1. OG

Observing ergodicity breaking via violations of random matrix theoretic predictions — •Venelin Pavlov[1], Peter Ivanov[1], Diego Porras[2], and Charlie Nation[3] — [1]Center for Quantum Technologies, Department of Physics, St. Kliment Ohridski University of Sofia, James Bourchier 5 blvd, 1164 Sofia, Bulgaria — [2]Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom

Quantum many-body systems can exhibit distinct regimes where dynamics is either ergodic in the sense that it explores an extensive region of available state-space, or non-ergodic, where the dynamics may be restricted or localized. In this work we explore the ability to probe the ergodicity of dynamics via local observables, and use expected results from random matrix theory (RMT) as a benchmark for the ergodic regime. We explore the time evolution of the quantum Fisher (QFI) information in the presence of three different ergodicity breaking mechanisms in a non-integrable spin system, namely, as a consequence of transition to integrability, Many-Body Localization (MBL) and Quantum Many-Body Scars (QMBS). We show that it can be used as a potential witness for transition to non-ergodic behavior. In ergodic quantum systems the QFI exhibits an additional intermediate linear time scaling together with it's typical short-time and long-time quadratic scaling. We show that in all of the three ergodicity breaking scenarios the violation of the random matrix theory predictions leads to the vanishing of the intermediate linear time regime.

MO 31.3 Thu 17:00 Philo 1. OG

Analytical determination of multi-time correlation functions in quantum chaotic systems — •Yoana Chorbadzhiyska[1], Peter Ivanov[1], and Charlie Nation[2] — [1]Faculty of Physics, Sofia University "St. Kliment Ohridski", 5 James Bourchier Blvd, Sofia 1164, Bulgaria — [2]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom

The time-dependence of multi-point observable correlation functions are essential quantities in analysis and simulation of quantum dynamics. Open quantum systems approaches utilize two-point correlations to describe the influence of an environment on a system of interest, and in studies of chaotic quantum system, the out-of-time-ordered correlator (OTOC) is used to probe chaoticity of dynamics. In this work we analytically derive the time dependence of multi-point observable correlation functions in quantum systems from a random matrix theoretic approach, with the highest order function of interest being the OTOC. We find in each case that dynamical contributions are related to a simple function, related to the Fourier transform of coarse-grained wave-functions. We compare the predicted dynamics to exact numerical experiments in a spin chain for various physical observables. We comment on implications towards the emergence of Markovianity and quantum regression in closed quantum systems, as well as relate our results to known bounds on chaotic dynamics.

MO 32: Molecular Spectroscopy III

Time: Friday 11:00–13:00 Location: P 204

Invited Talk MO 32.1 Fri 11:00 P 204

Time-resolved photoelectron spectroscopy of polycyclic hydrocarbons in rare-gas clusters — •Leonie Werner, Ulrich Bangert, Sebastian Hartweg, Yilin Li, Arne Morlok, Felix Riedel, Frank Stienkemeier, and Lukas Bruder — Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Time-resolved photoelectron spectroscopy (TRPES) is a powerful tool for probing ultrafast molecular dynamics, yet its application to molecules embedded in condensed environments remains challenging. We address this by studying polycyclic aromatic hydrocarbons (PAHs) dissolved in liquid-helium and solid-argon clusters, enabling controlled variations of environmental interactions. Despite the surrounding medium, we achieve high energy resolution and resolve environment-dependent differences in the molecular dynamics. In a first demonstration, we investigated the ultraviolet-induced ultrafast internal conversion in tetracene which is building on our previous work on isolated tetracene molecules in the gas phase [1]. In the next step, we intend to extend this to a systematic study of various acene molecules.

[1] A. Scognamiglio et al., J. Chem. Phys. (2024), 161, 024302

MO 32.2 Fri 11:30 P 204

Solvent-dependent relaxation pathways in Liquid-Jet Time-Resolved Photoelectron Spectroscopy — •Filippo Aria[1], Alina Khodko[2], and Oleg Kornilov[1] — [1]Max-Born-Institut, Berlin, Germany — [2]Institute of Physics NAS of Ukraine, Kyiv, Ukraine

Successful engineering of biomimetic carbon-carbon photoswitches with quantum yields comparable to natural systems requires understanding how solvent environments govern their relaxation pathways. Here, we investigate the solvent-dependent excited-state lifetime of 4-dimethylamino-4'-nitrostilbene (DMANS), a benchmark push-pull photoswitch. The measurements were carried out using UV pump-XUV probe liquid-jet time-resolved photoelectron spectroscopy (LJ-TRPES) with harmonic selection via a time-delay compensated monochromator. This approach yields precise energetic shifts and lifetimes of the active excited state across a series of solvents of moderate to high polarity. The results enable assessment of ultrafast photoswitching efficiency, identification of potential long-lived dark states inaccessible to conventional optical techniques, and establish the mechanistic role of solvation in controlling switching performance. This work demonstrates XUV LJ-TRPES as an essential tool for characterizing ultrafast dynamics in both synthetic and biologically inspired molecular photoswitches.

MO 32.3 Fri 11:45 P 204

Photoelectron Photoion Multicoincidence Study of Micro-Solvated Bio-Relevant Molecules — •Brendan Wouterlood[1], Sitanath Mondal[1], Madhusree Roy-Chowdhury[2,3], Gustavo Garcia-Macias[2], Laurent Nahon[2], Frank Stienkemeier[1], and Sebastian Hartweg[1] — [1]Institute of Physics, University of Freiburg — [2]Synchrotron SOLEIL, St. Aubin, France — [3]Institute of Physics, University of Kassel

Studying biomolecular building blocks, such as the nucleobase thymine and its precursor, pyridine, in the gas phase allows detailed insights into energetics and dynamics at the molecular level. As in-vivo biomolecular systems exist in the condensed phase, studying complexes of these molecules with water gives greater insight into decay channels that are available in biological systems, while still allowing the application of typical gas phase experimental approaches. One such technique is electron-ion-ion coincidence spectroscopy, which allows for detailed identification of fragmentation pathways that occur at or above the double-ionisation threshold of molecules and complexes. Here, distinguishing different auto-ionisation processes, such as the non-local intermolecular Coulombic decay (ICD) and electron transfer mediated decay (ETMD), as well as the local Auger-Meitner decay is challenging. Identification of these pathways can be helped by the occurrence of intramolecular proton transfer reactions that stabilise complexes with dicationic moieties. Insight into these processes is important to the field of radiation chemistry since the production of low energy electrons can trigger reactions which damage biological material.

MO 32.4 Fri 12:00 P 204

Helium cluster-isolation spectroscopy of quinacridone — •Aleksandr Demianenko, Kaleb Strahringer, Sebastian Hartweg, and Frank Stienkemeier — Institute of Physics, University of Freiburg, Germany

Organic chromophores are essential components of organic solar cells, field-effect transistors, light-emitting diodes, and supramolecular organic semiconductors. Their electronic and vibrational energy levels play a central role in determining collective molecular behaviors, including charge transport, exciton motion, and self-assembly.

In this talk, I will present helium cluster isolation spectroscopy to study the chromophore quinacridone. Although mostly known as an organic dye, quinacridone also shows highly interesting properties in its aggregation. Since it is a prochiral molecule it can be seen as a chiral object when attached to surfaces, where it can either aggregate in homochiral linear chains or more complex heterochiral structures.

The superfluid helium environment can be seen as isotropic thus allowing the aggregation of quinacridone molecules as non-chiral objects. Additionally, the ultracold temperature of the helium nanodroplets restrict population to vibrational ground states and produces well-resolved spectra for both monomers and oligomers in a minimally perturbing ultracold matrix. By combining a wavelength-tunable nanosecond laser, we obtain high-resolution laser-induced fluorescence spectra. These are presented in comparison with spectra on surfaces and in organic solvents.

MO 32.5 Fri 12:15 P 204

IR spectroscopy of metal complexes tailored by electron

transfer reduction in an ion trap — •Philipp Weber[1], Maximilian Emil Huber[1], Jennifer Meyer[1], Katja Heinze[2], and Christoph Riehn[1] — [1]Fachbereich Chemie und Forschungszentrum OPTIMAS, Kaiserslautern, DE — [2]Department of Chemistry, Johannes Gutenberg Universtät Mainz, DE

Understanding intrinsic structural properties of photocatalysts based on renewable 3d metal centers is of central importance when exploring their molecular design and reactivity in various environments [1,2]. Infrared multi-photon photodissociation spectroscopy (IRMPD) was conducted with the FELIX free electron laser on a set of differently charged, isolated Mn, Fe and Co complex species, containing the tridendate ligand dgpy (di-guanidyl-pyridine). This ligand accomodates a wide variety of metal species in different oxidation states, however, gas-phase reduction of tricationic $[\mathrm{Mn^{III}(dgpy)_2}]^{3+}$ produces a monocationic complex, which differs significantly in reactive and spectroscopic characteristics from its isoelectronic $\mathrm{Fe^{II}}$ and $\mathrm{Co^{III}}$ congeners, yielding fragmentation of the ligand backbone and structural distortion, leading to IR shifts in the characteristic N=C region. Comprehensive electronic structure calculations (DFT) give strong evidence that this behavior is not caused by a reduction of the metal center but alludes to a reduction of the pyridine moiety of the (here non-innocent) ligand. [1] M.Huber, J.Meyer J. Am. Soc. Mass Spectrom. 2024, 35, 11, 2642-2649 [2] N.East, K.Heinze Inorg. Chem. 2022, 61, 37, 14616-14625

MO 32.6 Fri 12:30 P 204

Two-Dimensional Infrared Spectroscopy of the SURMOF Cu(Da-DBDC)

— •Claudia Gräve[1], Ana Claudia Fingolo[2], Julian Brückel[3], Luis Ignacio Domenianni[1], Jörg Lindner[1], Stefan Bräse[3], Christof Wöll[2], and Peter Vöhringer[1] — [1]Clausius-Institute, University of Bonn, 53115 Bonn — [2]IFG, Karlsruhe Institute for Technology, 76344 Eggenstein-Leopoldshafen — [3]IOC, Karlsruhe Institute for Technology, 76131 Karlsruhe

In recent years, many significant applications for metal-organic frameworks have emerged. [1] 2D-IR spectroscopy can be used to examine important processes for their catalytic application: intramolecular vibrational redistribution (IVR) and vibrational energy transfer (VET).

We investigate the COO stretching modes and the azide asymmetric stretching fundamental of the surface-mounted metal-organic framework (SURMOF) Cu(Da-DBDC). [2] For reference, we also measured its organic linker, Diazido-tolanedicarboxylic acid, in liquid THF.

In the pump-probe spectra of both samples, the diagonal excited state absorption signal of the azide fundamental blue-shifts with increasing delay because of the involvement of low-frequency modes. The kinetic traces of the linker show a fast and a slow component due to IVR and VET to the solvent, respectively. In the SURMOF, the fast component is nearly identical, while the slow one is accelerated. We attribute this to resonant excitation hopping within the solid lattice, causing canonical heating of the pump-probe focal volume.

[1] H. Furukawa *et al., Science* **2013**, *341*, 1230444. [2] J. Song *et al., Angew. Chem. Int. Ed.* **2023**, *62*, e202306155.

MO 32.7 Fri 12:45 P 204

IR Spectroscopy of Larger Pyrrole Cation Clusters ($\mathrm{Py}_n{}^+$): Evolution of Charge Resonance Interaction

— •Dashjargal Arildii and Otto Dopfer — Technische Universität Berlin, Berlin, Germany

Aside from π H-bonding, cation/anion-π, and π-π stacking interactions, the charge resonance (CR) is a fundamental and strong force in charged arene dimers. In aromatic dimer cations, the positive charge is shared between the molecules depending on their ionization energy differences. Previously, we demonstrated a new high-resolution experimental approach (utilizing infrared photodissociation spectroscopy (IRPD)) to precisely probe the charge distribution and the CR interaction in aromatic dimer cations for the prototypical case of the pyrrole dimer cation ($\mathrm{Py}_2{}^+$) in the gas phase. Our further approach focuses on exploring the evolution of charge delocalization in larger $\mathrm{Py}_n{}^+$ (n>2) clusters. Hence, herein, we produce the $\mathrm{Py}_n{}^+$ (n=3-7) and their colder Ar-tagged $\mathrm{Py}_n{}^+\mathrm{Ar}$ (n=3-6) clusters in the supersonic plasma expansion and determine the structures by IRPD and computational approaches by analyzing the structure-sensitive NH stretch frequencies of $\mathrm{Py}_n{}^+$. The analysis of IRPD spectra of mass-selected $\mathrm{Py}_n{}^+$(Ar) with geometric parameters of intermolecular structures reveals that $\mathrm{Py}_n{}^+$ grows through solvating of CR-stabilized $\mathrm{Py}_2{}^+$ by additional Py ligands through the formation of NH...π H-bonds rather than by sharing the positive charge in the $\mathrm{Py}_n{}^+$ units.