

Molecular Physics Division Fachverband Molekülphysik (MO)

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Overview of Invited Talks and Sessions

(Lecture halls HS XV and HS XVI; Poster Tent)

Invited Talks

MO 1.1	Mon	11:00–11:30	HS XVI	Tracking and Controlling Chirality — ●DANIEL REICH
MO 18.1	Wed	14:30–15:00	HS XVI	Cold and Controlled Reactive Collisions — ●JOLIJN ONVLEE
MO 23.1	Thu	11:00–11:30	HS XV	Pickup and reactions of molecules on clusters relevant for atmospheric processes — ●JOZEF LENGYEL
MO 25.1	Thu	14:30–15:00	HS XVI	In good neighborhood: Suppression of radiation damage to X-ray-ionized molecules by intermolecular decay — ●ANDREAS HANS, DANA BLOSS, MADHUSREE ROY CHOWDHURY, CATMARN KÜSTNER-WETEKAM, FLORIAN TRINTER, ALEXANDER KULEFF, LORENZ S. CEDERBAUM, ARNO EHRESMANN
MO 29.1	Fri	11:00–11:30	HS XV	N₂ activation by transition metal clusters — MAX LUCZAK, CHRISTOPHER WIEHN, DANIELA FRIES, NIELS WOLFGRAMM, CHRISTOPH VAN WÜLLEN, ●GEREON NIEDNER-SCHATTEBURG

Invited Talks of the joint Symposium Molecular Spectroscopy of Liquid Jets (SYML)

See SYML for the full program of the symposium.

SYML 1.1	Mon	11:00–11:30	HS 1+2	The challenging road to work function measurements from aqueous solutions — ●BERND WINTER
SYML 1.2	Mon	11:30–12:00	HS 1+2	Liquid Delivery Systems for Time Resolved X-ray Spectroscopy — ●ZHONG YIN
SYML 1.3	Mon	12:00–12:30	HS 1+2	UV photoelectron spectroscopy of aqueous solutions — ●HELEN FIELDING, JOHANNA RADEMACHER, KATE ROBERTSON, EDOARDO SIMONETTI
SYML 1.4	Mon	12:30–13:00	HS 1+2	Decoherence and electron transport in liquid water observed with attosecond interferometric spectroscopy — ●HUGO MARROUX ET AL

Invited Talks of the joint Symposium SAMOP Dissertation Prize 2025 (SYAD)

See SYAD for the full program of the symposium.

SYAD 1.1	Mon	14:30–15:00	HS 1+2	A simple method to separate single- from multi-particle dynamics in time-resolved spectroscopy — ●JULIAN LÜTTIG
SYAD 1.2	Mon	15:00–15:30	HS 1+2	Time-resolving quantum dynamics in atoms and molecules with intense x-ray lasers and neural networks — ●ALEXANDER MAGUNIA
SYAD 1.3	Mon	15:30–16:00	HS 1+2	How rotation shapes the decay of diatomic carbon anions — ●VIVIANE C. SCHMIDT
SYAD 1.4	Mon	16:00–16:30	HS 1+2	Interstellar stardust from stellar explosions recorded in a deep-ocean ferromanganese crust within the last 10 million years — ●DOMINIK KOLL

Invited Talks of the joint Symposium Polaritonic Effects in Molecular System (SYPE)

See SYPE for the full program of the symposium.

SYPE 1.1	Tue	11:00–11:30	HS 1+2	Ab initio quantum electrodynamics: from microscopic details to thermodynamics — ●MICHAEL RUGGENTHALER
SYPE 1.2	Tue	11:30–12:00	HS 1+2	Ultrafast coherent exciton dynamics mediated by field-matter couplings — ●ANTONIETTA DE SIO
SYPE 1.3	Tue	12:00–12:30	HS 1+2	Open system dynamics for non-radiative transitions in molecules — ●CLAUDIU GENES
SYPE 1.4	Tue	12:30–13:00	HS 1+2	Strong light-matter coupling: from self-hybridized polaritons to Casimir self-assembly — ●TIMUR SHEGAI

Invited Talks of the joint Symposium Quantum Science and more in Ghana and Germany (SYGG)

See SYGG for the full program of the symposium.

SYGG 1.1	Tue	11:00–11:05	WP-HS	Welcome Adress — ●BIRGIT MÜNCH
SYGG 1.2	Tue	11:05–11:20	WP-HS	Quantum Education in Ghana — ●DORCAS ATTUABEA ADDO
SYGG 1.3	Tue	11:20–11:45	WP-HS	Mathematical and Computational Physics Research In Ghana: To Cultivate a Knowledge-Based and Sustainable Development Economy — ●HENRY MARTIN, HENRY ELORM QUARSHIE, MARK PAAL, FRANCIS KOFI AMPONG, ERIC KWABENA KYEH ABAVARE, MATTEO COLANGELI, ALESSANDRA CONTINENZA, JAIME MARIAN
SYGG 1.4	Tue	11:45–12:10	WP-HS	Forecasting the Economic Health of Ghana Using Quantum-Enhanced Long Short-Term Memory Model — ●PETER NIMBE, HENRY MARTIN, DORCAS ATTUABEA ADDO, NICODEMUS SONGOSE AWARAYI
SYGG 1.5	Tue	12:10–12:40	WP-HS	Quantum Technology with Spins — ●JOERG WRACHTRUP
SYGG 1.6	Tue	12:40–13:00	WP-HS	Renewable Energy Technologies for Rural Ghana: The Role of Appropriate Technology for Tailored solutions — ●MICHAEL KWEKU EDEM DONKOR

Prize and Invited Talks of the joint Awards Symposium (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	14:30–15:10	HS 1+2	A journey in mathematical quantum physics — ●REINHARD F. WERNER
SYAS 1.2	Thu	15:10–15:50	HS 1+2	Precision Tests of the Standard Model at Low Energies Using Stored Exotic Ions in Penning Traps — ●KLAUS BLAUM
SYAS 1.3	Thu	15:50–16:30	HS 1+2	Controlling light by atoms and atoms by light: from dark-state polaritons to many-body spin physics — ●MICHAEL FLEISCHHAUER
SYAS 1.4	Thu	16:30–16:35	HS 1+2	Quantum history at your fingertips: Launch of the DPG's Quantum History Wall — ●ARNE SCHIRRMACHER

Invited Talks of the joint Symposium Laser-Cooled Molecules (SYLC)

See SYLC for the full program of the symposium.

SYLC 1.1	Fri	11:00–11:30	HS 1+2	Measuring the electron electric dipole moment with laser-cooled molecules — ●MICHAEL TARBUTT
SYLC 1.2	Fri	11:30–12:00	HS 1+2	Laser-cooling of molecules in various charge states — ●ROBERT BERGER
SYLC 1.3	Fri	12:00–12:30	HS 1+2	Progress in quantum gases of polar molecules: Collisions, laser cooling, and trapping techniques — MARA MEYER ZUM ALTEN BORGLOH, JULE HEIER, BARAA SHAMMOUT, FRITZ VON GIERKE, TIMO POLL, JULIUS NIEDERSTUCKE, PAUL KAEBERT, SEBASTIAN ANSKEIT, JAKOB STALMANN, LEON KARPA, MIRCO SIERCKE, ●SILKE OSPELKAUS
SYLC 1.4	Fri	12:30–13:00	HS 1+2	Progress in laser cooling the AlF molecule — ●SIDNEY WRIGHT

Invited Talks of the joint Symposium New Avenues in Molecular Alignment and Orientation (SYAO)

See SYAO for the full program of the symposium.

SYAO 1.1	Fri	14:30–15:00	HS 1+2	Ultralong-range Rydberg molecules: Rotational hybridization, control of alignment and orientation, and Rydberg blockade — ●ROSARIO GONZÁLEZ-FÉREZ
SYAO 1.2	Fri	15:00–15:30	HS 1+2	Quantum control of molecular rotation — ●DOMINIQUE SUGNY
SYAO 1.3	Fri	15:30–16:00	HS 1+2	Strong-Field Ionization and Electron Rescattering Probabilities in the Molecular Frame — ●JOCHEN MIKOSCH, MARTIN GARRO, NARAYAN KUNDU, HORST ROTTKE, KILLIAN DICKSON, VARUN MAKHIJA, FEDERICO BRANCHI, FELIX SCHELL, MARK MERO, C P SCHULZ, SERGUEI PATCHKOVSKII, MARC VRAKKING
SYAO 1.4	Fri	16:00–16:30	HS 1+2	Coherent rotational control of gas phase molecular dipoles by concerted Terahertz and Near-IR pulses — ●SHARLY FLEISCHER

Sessions

MO 1.1–1.8	Mon	11:00–13:15	HS XVI	Chirality
MO 2.1–2.8	Mon	11:00–13:00	HS XV	Polaritonic Effects in Molecular Systems I (joint session MO/Q)
MO 3.1–3.7	Mon	11:00–12:45	HS I	Rydberg Atoms, Ions, and Molecules (joint session Q/MO)
MO 4.1–4.4	Mon	17:00–18:00	HS XVI	Molecular Spectroscopy of Liquid Jets I
MO 5.1–5.8	Tue	11:00–13:00	HS XVI	Ultrafast Dynamics I
MO 6.1–6.8	Tue	11:00–13:00	HS XV	Molecular Spectroscopy of Liquid Jets II
MO 7.1–7.5	Tue	11:00–12:30	GrHS Mathe	Attosecond Physics I (joint session A/MO)
MO 8.1–8.6	Tue	11:00–12:45	HS V	Strong-Field and Ultrafast Phenomena (joint session Q/MO)
MO 9.1–9.5	Tue	14:00–16:00	Tent	Poster – Novel Approaches
MO 10.1–10.4	Tue	14:00–16:00	Tent	Poster – Chirality
MO 11.1–11.6	Tue	14:00–16:00	Tent	Poster – Polaritonic Effects in Molecular Systems (joint session MO/Q)
MO 12.1–12.65	Tue	14:00–16:00	Tent	Poster – Cold Atoms and Molecules, Matter Waves (joint session Q/A/MO)
MO 13.1–13.8	Wed	11:00–13:00	HS XVI	Ultrafast Dynamics II
MO 14.1–14.8	Wed	11:00–13:00	HS XV	Polaritonic Effects in Molecular Systems II (joint session MO/Q)
MO 15.1–15.7	Wed	11:00–12:45	GrHS Mathe	Interaction with VUV and X-ray Light I (joint session A/MO)
MO 16.1–16.4	Wed	11:00–13:00	HS I PI	In Memoriam of Hermann Haken (joint session Q/MO)
MO 17	Wed	13:15–14:15	HS 5	Members’ Assembly
MO 18.1–18.7	Wed	14:30–16:30	HS XVI	Cold Molecules and Cold Chemistry (joint session MO/Q)
MO 19.1–19.6	Wed	14:30–16:15	GrHS Mathe	Interaction with Strong or Short Laser Pulses I (joint session A/MO)
MO 20.1–20.22	Wed	17:00–19:00	Tent	Poster – Molecular Spectroscopy and Dynamics
MO 21.1–21.10	Wed	17:00–19:00	Tent	Poster – Interaction with Strong or Short Laser Pulses (joint session A/MO)
MO 22.1–22.8	Thu	11:00–13:00	HS XVI	Ultrafast Dynamics III
MO 23.1–23.8	Thu	11:00–13:15	HS XV	Cluster and Nanoparticles I (joint session MO/A)
MO 24.1–24.5	Thu	11:00–12:30	GrHS Mathe	Attosecond Physics II (joint session A/MO)
MO 25.1–25.7	Thu	14:30–16:30	HS XVI	X-ray Spectroscopy
MO 26.1–26.15	Thu	17:00–19:00	Tent	Poster – Cold Molecules (joint session MO/Q)
MO 27.1–27.3	Thu	17:00–19:00	Tent	Poster – Collisions, Scattering and Correlation Phenomena (joint session A/MO)
MO 28.1–28.7	Fri	11:00–12:45	HS XVI	Ultrafast Dynamics IV
MO 29.1–29.7	Fri	11:00–13:00	HS XV	Cluster and Nanoparticles II (joint session MO/A)
MO 30.1–30.7	Fri	14:30–16:15	HS XVI	Molecular Spectroscopy and Theoretical Approaches

Members' Assembly of the Molecular Physics Division

Wednesday 13:15–14:15 HS 5

MO 1: Chirality

Time: Monday 11:00–13:15

Location: HS XVI

Invited Talk

MO 1.1 Mon 11:00 HS XVI
Tracking and Controlling Chirality — ●DANIEL REICH — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

Chiral observables such as electronic or photoelectron circular dichroism emerge from a complex interplay of the nuclear geometry, the initial state, and the interaction with the driving field. In order to understand and control chiral signatures it is imperative to identify and characterise the key ingredients among this trifecta. In this talk I demonstrate that chirality measures can be used as a tool to track the emergence and predict the strength of chiral observables. Furthermore, I highlight the role of the vibrational degree of freedom on the anisotropy observed for weakly allowed electronic transitions in chiral ketones. I show how the lessons learned from these and related results may serve as important puzzle pieces for quantum control of chiral observables.

MO 1.2 Mon 11:30 HS XVI
Robust chiral optical force via electric dipole interactions, inspired by a sea creature — ●ROBERT P CAMERON¹, DUNCAN McARTHUR¹, ALISON M YAO¹, NICK VOGLEY², and DAQING WANG² — ¹SUPA and Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom — ²Institute of Applied Physics, University of Bonn, 53115 Bonn, Germany

Inspired by a sea creature, we identify a robust chiral optical force that pushes the opposite enantiomers of a chiral molecule towards regions of orthogonal linear polarization in an optical field via electric dipole interactions. Our chiral optical force can be orders of magnitude stronger than others proposed to date and applies to essentially all chiral molecules, including isotopically chiral varieties which are notoriously difficult to separate using existing methods. We propose a realistic experiment supported by full numerical simulations, potentially enabling optical separation of opposite enantiomers for the first time.

MO 1.3 Mon 11:45 HS XVI
Chiral Selector Ion Vibrational Spectroscopy on Amino Acid Enantiomers — ●FRANCINE HORN¹, SONJA SCHMAHL², JIAYE JIN², and KNUT R. ASMIS² — ¹Leipzig University / Fritz Haber Institute — ²Leipzig University

The stereochemistry and conformational flexibility of chiral molecules have a strong impact on their biochemical, and pharmacological properties. A central analytical challenge is the generally applicable differentiation of enantiomers, as well as the fast and accurate determination of the enantiomeric excess. Gas phase vibrational action spectroscopy is a highly sensitive, selective, and fast tool for this purpose.

Chiral ionic analytes are transferred into the gas phase, where they interact with volatile chiral selector molecules under the formation of diastereomeric complexes. These are then mass-selected, cryogenically cooled, messenger-tagged and an infrared photodissociation (IRPD) spectrum is measured. The spectra of the vibrationally cold diastereomers exhibit sufficiently different IR fingerprints, such that they can be spectrally distinguished and quantified.

Different intermolecular non-covalent interactions can be present in diastereomers, among them H-bonds, π - π interactions and steric hindrance. We study a set of different chiral selector molecules and chiral amino acid analytes with different structural motifs to identify the decisive interactions in the present complexes. We aim at maximizing the differences in the vibrational action spectra of the diastereomers and gain insights into the interactions governing chiral recognition by characterizing the molecular level forces at work.

MO 1.4 Mon 12:00 HS XVI
the study of photoelectron circular dichroism in the ionization of (R) - (-) -fenchone by femtosecond laser — ●WENTAO CHEN¹, BRENDAN WOUTERLOO¹, CHIE NAKAYAMA², LUKAS BRUDER¹, SEBASTIAN HARTWEG¹, TAKAMASA MOMOSE², and FRANK STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg, 79104 Freiburg — ²University of British Columbia, Department of Chemistry, 2036 Main Mall, Vancouver BC, Canada

Photoelectron circular dichroism (PECD) is an intense chiroptical effect when chiral molecules are ionized by circularly-polarized light

(CPL). It would show a forwards/backward asymmetry in photoelectron angular distribution with respect to the CPL propagation direction and be several orders of magnitude more intense than traditional circular dichroism (CD) methods. As it's high sensitivity, PECD could be a fine tool for chirality identification. Here we aim to study the time-resolved PECD effect of (R)-(-)-Fenchone in helium droplets. In the beginning, we used CPL 400nm laser to ionized the Fenchone which is seeded in helium beam and detected the photoelectron by velocity map imaging method. We detected a significant PECD effect after subtracting the signals ionized by CPL lasers at different helicity. Then we will apply linear-polarized 200nm pump laser and CPL 266nm probe laser together with helium droplets method to study the time-resolved PECD effect in (R)-(-)-Fenchone. This will help us to figure out how the helium-droplets environment influences the ultrafast relaxation dynamics in chiral systems.

MO 1.5 Mon 12:15 HS XVI
Electron correlation in circular dichroism and chirality-induced spin selectivity — ●RAOUL M. M. EBELING¹, MAURICE BÉRINGUIER¹, VLADIMIRO MUJICA², DANIEL M. REICH¹, and CHRISTIANE P. KOCH¹ — ¹Freie Universität Berlin, Berlin, Germany — ²Arizona State University, Arizona, United States of America

We study two phenomena related to the interaction of chiral molecules with circularly polarized light, absorption circular dichroism (CD), and chirality-induced spin selectivity (CISS). We investigate both phenomena in chiral hydrogen and chiral helium, two model systems into which we introduce chirality via an artificial chiral potential. The chiral potential is constructed from a superposition of spherical harmonics and it can be interpreted as a way to mimic the chiral environment of a real molecule. Alternatively, our chiral hydrogen and chiral helium models could even be experimentally realized by placing the atoms in a setup involving several electric fields. By quantifying the chirality of the states with a suitable measure, we study the relationship between the chirality of the states and the CD and CISS. We investigate the influence of the strength of the chiral potential, the strength of the spin-orbit coupling, and the strength of the electron-electron interaction on both CD and CISS.

MO 1.6 Mon 12:30 HS XVI
Chirality induced spin polarization in one-photon ionization by circularly polarized light — ●PHILIP CAESAR FLORES¹, STEFANOS CARLSTROM¹, SERGUEI PATCHKOVSKI¹, ANDRES ORDONEZ^{2,3}, and OLGA SMIRNOVA^{1,4,5} — ¹Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — ²Department of Physics, Imperial College London, SW7 2BW London, United Kingdom — ³Department of Chemistry, Queen Mary University of London, E1 4NS London, United Kingdom — ⁴Technische Universität Berlin, 10623 Berlin, Germany — ⁵Technion, Israel Institute of Technology, 3200003, Haifa, Israel

Geometric magnetism controls the degree of enantiosensitive response in photoionization of chiral molecules and leads to new extremely efficient enantiosensitive observables (Commun. phys. 6, 2023, 257). Here, we show that the same phenomenon is responsible for: (i) spin-resolved enantiosensitive molecular orientation in photoionization, and (ii) spin-polarization of photoelectrons ejected from atoms and chiral molecules by circularly polarized fields. Our results provide a missing fundamental link between chirality and spin-polarization, and demonstrate that the coupling of geometric field to spin leads to high spin-polarization, which can be achieved even for very small spin-orbit interaction. Our conclusions are illustrated for synthetic chiral matter. We perform *ab initio* simulations of spin dynamics in photoionization of Argon atom using fully coupled spin-orbit code (Phys. Rev. A 106, 2022, 042806), and construct chiral superpositions of electronic states in Argon to quantify the link between chirality and spin-polarization in chiral targets.

MO 1.7 Mon 12:45 HS XVI
Models for Predicting Parity Violating Energy Differences in Chiral Molecules — ●NAMRATA GOHAIN and ROBERT BERGER — Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg

The weak interaction, unlike the other fundamental forces, violates parity and renders all atoms to be inherently chiral. However, this

effect becomes more pronounced in chiral molecules, leading to a tiny parity violating energy difference[1,2]. As attempts are being made to quantify the influence of parity violation in such molecules experimentally, one can also attempt to develop simplified models that predicts the energy difference between two enantiomers without explicit calculations. This can be advantageous for finding potential candidates that aids the development of high resolution spectroscopic techniques which can detect the parity violation in molecules[3]. In this contribution we will present one such model by focusing on different unsaturated chiral compounds as our candidates.

[1] M. Quack, *Angew. Chem. Int. Ed. Engl.*(1989), 28, 571-586.

[2] R. Berger and J. Stohner, *WIREs Comput Mol Sci.* (2019), 9, e1396.

[3] M. Quack, G. Seyfang and G. Wichmann, *Chem. Sci.* (2022), 13, 10598-10643

MO 1.8 Mon 13:00 HS XVI

Predicting splittings due to the weak interaction in rotational spectra of chiral clusters containing heavy elements —

•MIHNEA MĹAK-MĂRGINEAN and ROBERT BERGER — Philipps University of Marburg, 35032 Marburg, Germany

Rotational lines of chiral molecules are predicted to be split into those for left- and those for right-handed molecules when the fundamental weak interaction is taken into account. A successful detection of these tiny splittings would demonstrate parity nonconservation in the realms of molecular physics [1]. We aim at the prediction of such splittings in clusters containing heavy elements, which give rise to particularly promising effects. We use an implementation [2] of the zeroth order regular approximation to optimise the ground state electronic wave function of our systems, since relativity and spin-orbit coupling play a major role. Weak interaction contributions are accounted for perturbatively [3], with derivatives of these contributions with respect to atomic coordinates being computed analytically [4]. The latter are crucial for an efficient prediction within a rotation-vibration perturbation theory framework [5]. We will present general trends for the splittings and discuss their origin as well as prospects for the measurements.

[1] Berger, Stohner, *WIREs Comput. Mol. Sci.* 2019, 9, e1396.

[2] van Wüllen, *JCP* 1998, 109, 392, *ZPC* 2010, 224, 413.

[3] Berger, van Wüllen, *JCP* 2005, 122, 134316; Gaul, Berger, *JCP* 2020, 152, 044101.

[4] Brück, Sahu, Gaul, Berger, *JCP* 2023, 158, 194109.

[5] Riley, Raynes, Fowler, *Mol. Phys.* 1979, 38, 877.

MO 2: Polaritonic Effects in Molecular Systems I (joint session MO/Q)

Time: Monday 11:00–13:00

Location: HS XV

MO 2.1 Mon 11:00 HS XV

Changes in excimer properties under collective strong coupling — •MATTEO CASTAGNOLA, MARCUS TAKVAM LEXANDER, and HENRIK KOCH — Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway

The interplay between the local molecular dynamics and the collective polaritonic excitation is a fundamental but challenging aspect of polaritonic chemistry. While light-matter strong coupling has been proven to affect chemical properties, the underlying mechanism is still unclear. We employ a recently developed electronic-structure method for collective strong coupling to study the argon excimer, providing a simple prototype for a more general discussion on excimer properties. The computed potential energy surface exhibits a region where electronic, nuclear, and photonic degrees of freedom are strongly intertwined, and we analyze their coupling. Collective strong coupling produces an abrupt transition in the excited state's vibrational landscape, causing the higher vibrational levels to behave similarly to the ground state vibrations. We thus find that collective strong coupling inhibits the formation of the excimer once the collective coupling exceeds a critical value. We propose this is a general feature of excimers under collective strong coupling, which could be investigated by recording absorption and emission spectra, offering an additional facet of polaritonic chemistry.

MO 2.2 Mon 11:15 HS XV

Quantized embedding approaches for collective strong coupling – and what about Coulomb? — FRIEDER LINDEL^{1,2}, DOMINIK LENTRODT², STEFAN BUHMANN³, and •CHRISTIAN SCHÄFER⁴ — ¹Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ²Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — ³Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ⁴Department of Physics, Chalmers University of Technology, 41296 Göteborg, Sweden

Collective light-matter interactions have been used to control chemistry and energy transfer, yet accessible approaches that combine ab initio methodology with large many-body quantum optical systems are missing due to the fast increase in computational cost for explicit simulations. We introduce such an accessible ab initio quantum embedding concept for many-body quantum optical systems that allows us to treat the collective coupling of molecular many-body systems effectively in the spirit of macroscopic quantum electrodynamics while keeping the rigor of ab initio quantum chemistry for the molecular structure [1]. We illustrate the underlying assumptions by comparison to the Tavis-Cummings model and highlight the importance of Coulombic interactions between emitter and solvent molecules, as well as their potential interplay in collective strong coupling [2].

[1] *J. Chem. Phys.* 161, 154111 (2024). [2] *J. Phys. Chem. Lett.*

2024, 15, 1428-1434.

MO 2.3 Mon 11:30 HS XV

Simulation of polaritons in real cavities through a semiclassical approach — •CARLOS BUSTAMANTE¹, FRANCO BONAFÉ¹, MICHAEL RUGGENTHALER¹, MAXIM SUKHAREV², ABRAHAM NITZAN³, and ANGEL RUBIO¹ — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²Department of Physics, Arizona State University, Tempe, Arizona, USA — ³Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania, USA

The strong coupling between light and matter reached within optical cavities has opened a new path to modify material properties and chemical reactions. For chemical effects, this strong coupling condition may be achieved when the photonic modes of the cavity resonate with molecular vibrations or electronic transitions, leading to vibrational strong coupling (VSC) and electronic strong coupling (ESC) respectively, creating a hybrid state between light and matter called polaritons. Although this research area is rapidly expanding, the simulation of a realistic experimental setup, capturing all relevant factors, remains a challenge. Our study proposes a semiclassical approach involving the propagation of Maxwell equations on a grid, while incorporating tens to hundreds of molecules using the quantum mechanical simulation software DFTB+. By modelling the mirrors with the Drude permittivity, we can integrate them into the setup to emulate a Fabry-Perot cavity. Our results demonstrate that our setup can accurately represent various experimental observations, including Rabi-splitting and collective effects.

MO 2.4 Mon 11:45 HS XV

Analytic model reveals local molecular polarizability changes induced by collective VSC — •JACOB HORAK^{1,2}, DOMINIK SIDLER^{1,2,3}, THOMAS SCHNAPPINGER⁴, MICHAEL RUGGENTHALER^{1,2}, and ANGEL RUBIO^{1,2,5} — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — ³Paul Scherrer Institut, Villigen, Switzerland — ⁴Stockholm University, Stockholm, Sweden — ⁵The Flatiron Institute, New York, USA

Despite recent numerical evidence, one of the fundamental theoretical mysteries of polaritonic chemistry is how and if collective strong coupling can induce local changes of the electronic structure to modify chemical properties. Here we present non-perturbative analytic results for a model system consisting of an ensemble of N harmonic molecules under vibrational strong coupling (VSC) that alters our present understanding of this fundamental question. We discover that the electronic molecular polarizabilities are modified even in the case of vanishingly small single-molecule couplings. Consequently, this non-perturbative local polarization mechanism persists even in the large- N limit. In contrast, a perturbative calculation of the polarizabilities leads to a

qualitatively erroneous scaling behavior with vanishing effects in the large- N limit. Our fundamental theoretical observations demonstrate that hitherto existing collective-scaling arguments are insufficient for polaritonic chemistry / physics.

MO 2.5 Mon 12:00 HS XV

Polaritonic Molecular Orbitals — ●YASSIR EL MOUTAOUKAL — Norwegian University of Science and Technology, 7491 Trondheim, Norway

A comprehensive understanding of electron-photon correlation is essential for describing the reshaping of molecular orbitals in quantum electrodynamics (QED) environments.

The strong coupling QED Hartree-Fock (SC-QED-HF) theory tackles these aspects by providing consistent molecular orbitals in the strong coupling regime. The previous implementation, however, displays significant convergence issues.

In this talk I present how these limitations can be overcome by capturing the coupling between the electron-photon dressing parameters, enhancing the modeling of large molecular systems coupled to electromagnetic vacuum fluctuations.

The development of more correlated methods and response theory using the SC-QED-HF reference wavefunction are now possible and currently in development, as well as the extension to a multi-mode Hamiltonian and chiral cavities.

MO 2.6 Mon 12:15 HS XV

Higher excitations manifolds in the Tavis-Cummings model for multi-level systems — ●LUCAS BORGES, THOMAS SCHNAP-PINGER, and MARKUS KOWALEWSKI — Department of Physics, Stockholm University, Stockholm, Sweden

The Tavis-Cummings model describes the interaction of multiple quantum emitters, such as atoms or molecules, with the quantized electromagnetic field modes of an optical cavity, leading to the emergence of polariton states (eigenstates of the coupled system). Most studies focus on the first excitation manifold, which includes states with a single excitation (one photon or one excited atom). The polariton states within this manifold are well separated into bright and dark states.

However, molecular ensembles in a cavity may carry multiple excitations, thus requiring the inclusion of higher excitation manifolds. We present a study of a system of N three-level systems coupled to a single lossy cavity mode, truncating the Hamiltonian to the N th excitation manifold. The system models a molecular ensemble, where two levels are directly coupled to the cavity, while the third level is weakly coupled to the second energy level. We show that when a fraction of the system's excitations initially reside in these third levels, the cavity mediates its decay to the ground state, revealing a new pathway influenced by the cavity dynamics.

MO 2.7 Mon 12:30 HS XV

Relativistic quantum electrodynamical density functional theory beyond ideal cavities — ●LUKAS KONECNY¹, MARK KAMPER SVENDSEN^{2,3}, VALERIA KOSHELEVA³, MICHAEL RUGGENTHALER³, and ANGEL RUBIO³ — ¹Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, UiT The Arctic University of Norway, Tromsø, Norway — ²NNF Quantum Computing Programme, Niels Bohr Institute, Copenhagen, Denmark — ³Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany

Quantum electrodynamical density functional theory (QEDFT) is one of the computational methods that combine quantum chemical treatment of matter with quantized description of light. This allows to describe the effect of strong coupling of matter to photonic modes while preserving the accuracy necessary for chemical and spectroscopic applications together with the favourable computational cost associated with density functional theory. Building on recently introduced relativistic QEDFT based on the four-component Dirac-Coulomb Hamiltonian we extend the methodology beyond idealized single-mode Fabry-Pérot cavities to the interaction with a quasi-continuum of photonic modes that enables the description of realistic cavities as well as radiative decay via the coupling to vacuum modes while the relativistic approach to electronic structure enables accurate treatment of heavy elements and effects of spin-orbit coupling such as singlet-triplet transitions. Thus we expand the applicability of QEDFT into new domains.

MO 2.8 Mon 12:45 HS XV

Impact of dipole self-energy on cavity-induced nonadiabatic dynamics — CSABA FÁBRI^{1,2}, GÁBOR J. HALÁSZ³, LORENZ S. CEDERBAUM⁴, and ●ÁGNES VIBÓK¹ — ¹HUN-REN-ELTE Complex Chemical Systems Research Group, Budapest, Hungary — ²Department of Theoretical Physics, Debrecen University, Debrecen, Hungary — ³Institute of Informatics, Debrecen University, Debrecen, Hungary — ⁴Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Heidelberg, Germany

The coupling of matter to the quantized electromagnetic field of a plasmonic or optical cavity can be harnessed to modify and control the chemical and physical properties of molecules. In optical cavities, a term known as the dipole self-energy (DSE) appears in the Hamiltonian to assure gauge invariance.

We study the impact of the DSE on cavity-induced nonadiabatic dynamics in a realistic system. For that purpose, various matrix elements of the DSE are computed as functions of the nuclear coordinates and the dynamics of the system after laser excitation is investigated. The cavity is known to induce conical intersections between polaritons, which gives rise to substantial nonadiabatic effects. The DSE is shown to slightly affect these light-induced conical intersections and, in particular, break their symmetry.

MO 3: Rydberg Atoms, Ions, and Molecules (joint session Q/MO)

Time: Monday 11:00–12:45

Location: HS I

MO 3.1 Mon 11:00 HS I

Interfacing Rydberg atoms with an GHz electromechanical oscillator — ●JULIA GAMPER, CEDRIC WIND, VALERIE MAUTH, SAMUEL GERMER, WOLFGANG ALT, and SEBASTIAN HOFFERBERTH — Institute of Applied Physics, University of Bonn, Germany

Rydberg atoms exhibit strong electric dipole transitions over a large range of the electromagnetic spectrum which make them interesting for hybrid quantum systems bridging vastly different frequency regimes.

In this talk, I will present our approach to interfacing optically controlled Rydberg atoms with an electromechanical oscillator for cooling one of the vibrational modes of the oscillator to its quantum mechanical ground state by exchange of microwave photons with the atoms.

I will discuss the design of this hybrid system and present our progress on the construction. Our system consists of a 3D magneto-optical trap for loading rubidium atoms which are subsequently magnetically transported to the experimental region which is at cryogenic temperatures of 4K and includes a vibration-isolation system that reduces vibrations below 25nm.

As a first step towards our envisioned hybrid system, we plan to trap the rubidium atoms with a superconducting wire trap on a chip with an integrated microwave resonator to drive microwave transitions

of the Rydberg atoms close to the cryogenic surface.

MO 3.2 Mon 11:15 HS I

Magic wavelength traps for collective Rydberg excitations — ●DANIIL SVIRSKIY¹, LUKAS AHLHEIT¹, CHRIS NILL², JAN DE HAAN¹, NINA STIESDAL¹, WOLFGANG ALT¹, IGOR LESANOVSKY², and SEBASTIAN HOFFERBERTH¹ — ¹Institute of Applied Physics, University of Bonn, Germany — ²Institute of Theoretical Physics, University of Tübingen, Germany

Storage of optical photons as collective excitation in an ultracold atomic medium is one of the possible candidates for the realization of a quantum memory. However, photon storage times are limited by various decoherence mechanisms, including thermal atomic motion and inhomogeneous differential light shifts between atoms sharing the excitation. The latter can be suppressed by magic trapping, which equalizes the AC Stark shifts for the ground and excited levels of the atom.

In this talk, I present our implementation of a magic trap for ultracold Rydberg atoms. We conduct photon storage and retrieval measurements for two different trapping geometries: a magic lattice and a running wave trap with different trap wavelengths. Our experiments

demonstrate that both the longitudinal standing wave and the radial trap shape impact the magic condition. This difference arises from the Rydberg electron wavefunction extending over a significant region of the trap potential and contributing a ponderomotive part to the trap potential. We investigate how this part scales with principle quantum number n and determine the optimal magic lattice wavelength for each Rydberg state.

MO 3.3 Mon 11:30 HS I

Avoided-Crossing Rydberg Facilitation with Phonon Coupling in 1D Lattices — •DANIEL BRADY and MICHAEL FLEISCHHAUER — RPTU Kaiserslautern, Kaiserslautern, Germany

Rydberg anti-blockade (facilitation) offers one of the most promising mechanisms for realizing robust neutral-atom quantum gates. However, concomitant with the strong dipolar interactions between Rydberg atoms (spins) are mechanical forces coupling Rydberg atoms to high motional states (phonons) in their respective tweezer traps. This has so far kept experimental realizations of quantum gates with facilitation out of reach. Recently, Rydberg excitations have been created by coupling to an avoided-crossing potential in an experimental setting. This approximately harmonic potential alters the nature of the spin-phonon coupling and therefore might offer a method of realizing quantum gates.

For a chain of atoms trapped in tweezer arrays under the facilitation constraint, we numerically simulate the dynamics of the spin-phonon coupling. In particular we investigate how the motional degrees of freedom affect the spreading dynamics of Rydberg excitations.

MO 3.4 Mon 11:45 HS I

Electronically Excited Cold Rydberg Ion Crystals — •MARION MALLWEGER¹, NATALIA KUK¹, HARRY PARKE¹, IVO STRAKA¹, ROBIN THOMM¹, VINAY SHANKAR¹, WEIBIN LI³, IGOR LESANOVSKY^{2,3}, and MARKUS HENNRICH¹ — ¹Stockholm University, Stockholm, Sweden — ²Institut für Theoretische Physik, Universität Tübingen, Germany — ³School of Physics and Astronomy, University of Nottingham, United Kingdom

Trapped Rydberg ions harness two advantages: a well defined confinement through the charge of the ion and strong interactions through its large principle quantum number. In the experiments presented here a trapped strontium ion was excited from the metastable 4D to Rydberg states. While for the ground state of the ion, the polarizability is negligible, for Rydberg ions it increases as $\sim n^7$. Thus, the high polarizability of the Rydberg state with respect to the ground state leads to a change in radial confinement during the Rydberg excitation. For an ion crystal, this change can be enough to cause a structural phase transition from a linear configuration in the lower-lying electronic states to a zigzag configuration in the Rydberg state. We explore and characterize this electronic state dependent structural phase transition. We investigate this effect via spectroscopy scans of the Rydberg resonance with varying radial confinement close to the transition point of the zigzag crystal configuration. By tuning the polarizability, the change in radial trap confinement and therefore the transition point can be tuned. This enables a novel method for studying molecular phenomena with ions in the well-isolated environment of a Paul trap.

MO 3.5 Mon 12:00 HS I

Ultralong-Range Ytterbium Rydberg Molecules — •TANGI LEGRAND, FLORIAN PAUSEWANG, XIN WANG, LUDWIG MÜLLER, EDUARDO URUÑUELA, WOLFGANG ALT, and SEBASTIAN HOFFERBERTH — Institute of Applied Physics, University of Bonn, Germany

An ultralong-range Rydberg molecule forms through the interaction

between a ground-state atom and the electron of a highly excited Rydberg atom, leading to molecular states characterized by extreme spatial extension, large dipole moments and long lifetimes.

In this work, we present the spectroscopic characterization of such molecules in a dense and ultracold ytterbium (Yb) gas. Using two-photon excitation, we probe the molecular binding energies and map out the vibrational spectra. By applying low-energy quantum scattering techniques to the observed binding energies, we can extract the electron-neutral atom s -wave scattering length. Our data enables precise benchmarking of Yb model wavefunctions derived from multi-channel quantum defect theory, offering a robust validation for the accuracy of theoretical descriptions of Rydberg (molecular) states.

We also present our apparatus featuring a two-chamber compact design comprising a dispenser-loaded 2D MOT and a two-color 3D MOT allowing narrow-linewidth cooling. After loading into an optical trap, we reach $T < 10 \mu\text{K}$ at atomic densities of 10^{13} cm^{-3} . By consecutive evaporation we reach $T \approx 200 \text{ nK}$. Electrodes around the atomic cloud allow electric field background compensation, field ionization of Rydberg atoms and molecules, and their delivery to a microchannel plate.

MO 3.6 Mon 12:15 HS I

Roughening dynamics of quantum interfaces — WLADISLAW KRINITZIN^{1,2}, •NIKLAS TAUSENDPFUND^{1,3}, MATTEO RIZZI^{1,3}, MARKUS HEYL⁴, and MARKUS SCHMITT^{1,2} — ¹Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, Jülich, Germany — ²Faculty of Informatics and Data Science, University of Regensburg, Regensburg, Germany — ³Institute for Theoretical Physics, University of Cologne, Köln, Germany — ⁴Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The roughening transition, known from three-dimensional classical spin systems, describes how fluctuations of interfaces transition from being bounded to being extensive when crossing the characteristic roughening temperature. We explore signatures of such phenomena in the dynamics of domain walls in the two dimensional quantum Ising model, where we observe pre-thermal steady states in their evolution well beyond the perturbative limit using Tree Tensor Networks. We formulate an effective model of the interface, which captures qualitative features of a roughening transition. Most notably, it exhibits a Berezinskii-Kosterlitz-Thouless quantum phase transition from smooth to rough interfaces, whose signatures extend to finite temperatures. These findings can be related to the observed slow thermalization in the full model, opening the way to a better understanding of pre-thermalization effects in interface dynamics, which can be easily implemented and tested in experimental setups such as Rydberg atom experiments.

MO 3.7 Mon 12:30 HS I

Control thermalization in one dimensional Floquet driven Rydberg atom chain — •WEIBIN LI¹, YUNHUI HE², and JIANMING ZHAO² — ¹University of Nottingham, Nottingham, UK — ²Shanxi University, Taiyuan, China

We study Floquet thermalization of a one dimensional disorder-free Rydberg atom chain. The stroboscopic dynamics of the finite Rydberg atom chain is numerically solved. We show that the Floquet thermalization results from the emergence of an effective multi-body interaction across the atom chain. We characterize the properties of the thermalization using level spacing statistics and entanglement entropy. The dependence of the Floquet thermalization on the driving period and laser detuning is examined. The scaling with the system size and dependence on the initial state are explored. Our results can be readily observed in the current Rydberg atom array experiments.

MO 4: Molecular Spectroscopy of Liquid Jets I

Time: Monday 17:00–18:00

Location: HS XVI

MO 4.1 Mon 17:00 HS XVI

Development and implementation of a flat jet device for mesophase-dependent High Harmonic Generation experiments in thermotropic liquid crystals — •MARTA LUISA MURILLO-SÁNCHEZ, NATALIA COPETE-PLAZAS, and LAURA CATTANEO — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Deutschland

High harmonic generation (HHG) spectroscopy aims for the study of ultrafast molecular dynamics, offering insights into electronic and nuclear motion. While early work in gas-phase systems can be fully understood by the three-step model, the focus has shifted to condensed matter, where collective interactions make HHG mechanisms more complex to unravel. To explore these mechanisms, thermotropic liquid crystals (LCs) are promising due to their tunable mesophases*intermediate states between liquid and crystalline

phases*achieved via temperature changes. Using a custom flat jet device adapted for the high viscosity and non-Newtonian behavior of LCs, we generated stable, down to 2 μm -thin sheets for substrate-free HHG experiments with a precise temperature control. Preliminary HHG spectra were obtained for isotropic (liquid) and nematic phases of 4-cyano-4'-pentylbiphenyl (5CB) under a mid-infrared driving field (4 μm). Results highlighted the nematic phase*s anisotropic structure and birefringence, underscoring the need for molecular alignment control. These findings pave the way for optimizing HHG in LCs and deepening our understanding of nonlinear optical phenomena in soft condensed matter.

MO 4.2 Mon 17:15 HS XVI

Exploring the origin of multiple plateaus in liquid high-harmonic generation — ●ANGANA MONDAL¹, OFER NEUFELD², TADAS BALCIUNAS¹, ZHONG YIN¹, BENEDIKT WASSER¹, SERGE MÜLLER¹, ANGEL RUBIO^{3,4,5}, NICOLAS TANCOGNE-DEJEAN^{3,4}, and HANS JAKOB WÖRNER¹ — ¹Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — ²Technion Israel Institute of Technology, Israel — ³Max Planck Institute for the Structure and Dynamics of Matter, Germany — ⁴Center for Free-Electron Laser Science CFEL, DESY, Germany — ⁵Physics Department, University of Hamburg, Germany

Recent studies of liquid high-harmonic generation highlight scattering-limited electron trajectories as the key mechanism, with on-site recombination as the primary process[1]. However, this framework left unexplained the absence of higher-order nonlinearities with increasing laser power. Here we report, the observation of a second plateau in the liquid HHG spectrum, attributed to electron recombination with neighboring molecules, dominated by second solvation shell contributions via hole delocalization [2,3]. The plateau exhibits weak scaling with laser wavelength, intensity, and distinct ellipticity dependence, confirmed experimentally and theoretically. Our results predict the existence of higher-order plateaus linked to successive recombination events, establishing a pathway for attosecond-scale probing of electron dynamics in liquids and solutions. Reference 1. A Mondal et al. Nat. Phys. 19, 1813-1820 (2023) 2. I Jordan et al. Science 369, 974-979 (2020) 3. X Gong et al. Nature 609, 507-511 (2022)

MO 4.3 Mon 17:30 HS XVI

Delocalized electrons in aqueous jets — ●FABIO NOVELLI¹, ADRIAN BUCHMANN¹, IQRA YOUSAF¹, LION-LUCA STIEWE¹, WIBKE BRONCH², FEDERICO CILENTO², CLAUDIUS HOBERG¹, and MARTINA HAVENITH¹ — ¹Ruhr University Bochum, Bochum, Germany —

²Elettra - Sincrotrone Trieste S.C.p.A., Strada Statale 14, km 163.5, Trieste I-34149, Italy

The photoexcitation of iodide solutions serves as a model for generating electrons in liquid water. We used transient absorption spectroscopy across terahertz, near-infrared, and visible frequencies on a 10-micron thick liquid jet operating at normal temperature and pressure conditions (20 C, 1 atm). We demonstrate that the two-photon absorption of 400 nm pulses can impulsively generate short-lived (250 fs) electrons that are delocalized tens of angstroms away from the parent anion. These electron states are associated with 5p-6p transitions, similar to frustrated excitons with a large radius. Our transient terahertz spectroscopy findings reveal that delocalized electrons exhibit an electronic mobility of 1 cm²/(Vs). This is significantly higher, by approximately 500 times, than that of fully relaxed or hydrated electrons, and roughly comparable to that found in amorphous silicon or conductive conjugated polymers. This work highlights the effectiveness of transient terahertz spectroscopy in investigating low-energy, intra-band electronic transitions in soft condensed matter systems and can assist in the development of liquid-based optoelectronic devices.

MO 4.4 Mon 17:45 HS XVI

Optical-Pump THz-Probe Spectroscopy of Myoglobin in Water — ●ADRIAN BUCHMANN¹, SEBASTIAN JUNG¹, LION-LUCA STIEWE¹, LUIGI CAMINITI², and MARTINA HAVENITH¹ — ¹Ruhr Universität Bochum, Bochum, Germany — ²European Laboratory for Non-Linear Spectroscopy, Florence, Italy

Enzymes (functional proteins) are known to be the most effective catalysts. In the search for more and more effective catalysts and energy storage devices, chemists look for solutions to copy nature and attempt to design proteins from scratch. However, so far most fail to reproduce the catalytic activity of their evolved siblings. A factor suggested to contribute to this shortcoming is the unknown mechanism of energy flow through the proteins. We employ nonlinear THz spectroscopy to follow this energy flow from an excited heme through its surrounding myoglobin protein into the surrounding solvent. This enables us to determine the energy flow properties from the vibrational relaxation time of the protein. Optical Pump THz probe spectroscopy in water requires a windowless approach making the liquid jet essential for the experiment.

We observe a transient signal which reaches an equilibrium around 50 ps. The final difference spectrum resembles the spectrum of heated water with a temperature difference of 0.1 K. We can determine a rise time of 7.9 +/- 0.5 ps which is consistent with the vibrational relaxation time observed in the IR frequency range.

MO 5: Ultrafast Dynamics I

Time: Tuesday 11:00–13:00

Location: HS XVI

MO 5.1 Tue 11:00 HS XVI

Ultrafast Excited State Dynamics of the Nitrene Formation in Bis-Carbene-Ni/Pd/Pt-Azides — ●MARKUS BAUER¹, FREDERIK SCHERZ², LUIS IGNACIO DOMENIANNI¹, ANNA PAVUN³, BIPRAJIT SARKAR⁴, STEFAN HOHLOCH³, VERA KREWALD², and PETER VÖHRINGER¹ — ¹Clausius Institut für physikalische Chemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Deutschland — ²Fachbereich Chemie, Technische Universität Darmstadt, Deutschland — ³Department of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Österreich — ⁴Fachbereich Biologie, Chemie, Pharmazie, Freie Universität Berlin, Deutschland

Nitrenes are highly reactive subvalent nitrogen species that are often used as intermediates in many organic and pharmaceutical syntheses.

We investigated the UV-induced photochemistry of three square-planar metal-azides coordinated by a tridentate ligand possessing two carbene and one amido donor (Metal=Ni, Pd, Pt). Utilizing femtosecond UV-pump-mIR-probe and UV-pump-Vis-probe spectroscopy, we were able to record the primary photochemical processes following the UV-excitation, which differ significantly depending on the metal center. Furthermore, we succeeded in identifying the key intermediates preceding nitrene formation using quantum chemical calculations.

The nickel-based complex undergoes almost exclusively ground-state recovery (GSR) and seems to remain on the singlet surface, while both the palladium, as well as the platinum species exhibit complex, but distinct intersystem crossing dynamics. Additionally, the quantum yield

increases significantly with the mass of the metal center.

MO 5.2 Tue 11:15 HS XVI

Excited-state wavepacket dynamics of the photoredox catalyst Ti^{IV}(Cp)₂(NCS)₂ — ●JONAS SCHMIDT, LUIS IGNACIO DOMENIANNI, and PETER VÖHRINGER — Clausius-Institut für Physikalische und Theoretische Chemie, Bonn, Deutschland

Recently, we reported the observation of the entry events of Ti(Cp)₂(NCS)₂ into a photo-catalytic cycle in real-time. Using time-resolved mid-infrared spectroscopy, we identified the intermediate states involved and tracked the reductive quenching reaction of the active catalyst with a sacrificial amine electron donor over broad timescales, spanning from picoseconds to hundreds of microseconds.

Here, we report on the very early dynamics of the electronic relaxation of the locally excited singlet state, S₃. To this end, we employed ultra-fast near-UV-pump/white-light-probe spectroscopy with a time resolution of a few tens of femtoseconds. We could observe a prompt, structureless transient absorption ranging from 600 to 900 nm. On timescales below two picoseconds, the absorption exhibits coherent oscillations with a frequency of 140 cm⁻¹. An analysis of probe-wavelength dependence of their phase and amplitude provides evidence that they are due to vibrational wavepacket dynamics in the energetically lowest singlet excited state, S₁, of the complex. TDDFT suggests that the initial S₃-to-S₁ internal conversion creates a coherent superposition in the Cp-Ti-Cp bending vibration of S₁.

We are currently in the process of conducting complementary experiments on the fully methylated complex $\text{Ti}(\text{Cp})_2^*(\text{NCS})_2$ to verify this assignment.

MO 5.3 Tue 11:30 HS XVI

Ultrafast Light-Induced Dynamics of Competing Reaction Pathways in Molecular Rings — •VESNA ERIC¹, FRANCESCO MONTORSI^{1,2}, SIMONA DJUMAYSKA¹, and DANIEL KEEFER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²University of Bologna, Bologna, Italy

Conical intersections mediate ultrafast light-induced processes in molecular systems. Due to the strong coupling of electronic and nuclear degrees of freedom, conical intersections open channels for fast energy transfer between excited states. Recent theoretical studies reveal the potential of stimulated X-ray Raman spectroscopy to provide distinct spectral signals of the passage through conical intersections, which previously remained elusive. Here, we extend this concept towards spectrally distinguishing competing conical intersection-mediated pathways. We employ computational modelling to investigate the photochemistry of 2,5-dichlorofuran molecules exhibiting competing reaction pathways, ring puckering and opening, as typically observed in molecular ring structures. Our simulation protocol includes multireference (CASPT2) electronic structure calculations, quantum dynamics, and evaluation of stimulated X-ray Raman signals. Finally, we discuss the possibility of the spectral separation between the competing conical intersections by tuning the X-ray probe pulse to the pre-edge of the Carbon, Nitrogen and Oxygen transitions.

MO 5.4 Tue 11:45 HS XVI

Investigating Competing Photochemical Pathways in Furan-based systems via Surface Hopping and Ultrafast Electron Diffraction simulations — •SIMONA DJUMAYSKA, FRANCESCO MONTORSI, VESNA ERIC, and DANIEL KEEFER — Max Planck Institute for Polymer research, Mainz, Germany

Photochemical reactions at conical intersections (CIs) play a crucial role in determining the photoproducts of excited-state dynamics in molecular systems. Such is the case for systems like furan and its derivatives, which exhibit complex nonadiabatic dynamics influenced by these intersections. The photochemistry of furan involves two main competing pathways: ring-opening and ring-puckering. In this work, we used surface-hopping (SH) dynamics based on high-level CASPT2 calculations of the electronic structure to study these photochemical reactions. This approach allows us to simulate the motion of nuclei as they undergo non-adiabatic transitions between electronic states at CIs. To better interpret these results and connect them to experiments, we calculate ultrafast electron diffraction (UED) signals. We demonstrate how UED signals can differentiate between the ring-opening and ring-puckering motions. This study shows that combining SH dynamics with UED simulations is a useful way to investigate and distinguish photochemical processes in molecules like furan. Our simulations further help to predict and interpret cutting-edge UED experiments geared towards unraveling the interplay between nuclear motion and electronic transitions in excited states.

MO 5.5 Tue 12:00 HS XVI

Investigating the Ultrafast Molecular Relaxation of 4-Thiouracil Using Time-Resolved X-Ray Photoelectron Spectroscopy — •DENNIS MAYER¹, DAVID PICCONI², MATTEO BONANOMI^{3,4}, MILTCHO DANAILOV⁵, ALEXANDER DEMIDOVICH⁵, MICHELE DEVETTA⁴, MICHELE DI FRAIA⁵, DAVIDE FACCIALA⁴, RAIMUND FEIFEL⁶, CESARE GRAZIOLI⁷, FABIANO LEVER¹, NITSH PAL⁸, VASILIS PETROPOULOS³, KEVIN PRINCE⁵, OKSANA PLEKAN⁵, RICHARD SQUIBB⁶, CATERINA VOZZI⁴, GIULIO CERULLO^{3,4}, and MARKUS GÜHR^{1,9} — ¹DESY, Hamburg, Germany — ²Heinrich-Heine University, Düsseldorf, Germany — ³Politecnico di Milano, Italy — ⁴CNR-IFN, Milan, Italy — ⁵Eletra-Sincrotrone Trieste, Italy — ⁶University of Gothenburg, Sweden — ⁷CNR-IOM, Trieste, Italy — ⁸Heriot-Watt University, Edinburgh, UK — ⁹University of Hamburg, Germany

Recent experiments on 4-thiouracil observed different time constants for the UV-induced relaxation into its triplet state that go beyond the difference between experiments in the gas and solution phase [1,2]. Utilizing the element- and site-selectivity of x-rays, we studied the relaxation process 4-thiouracil using gas-phase time-resolved x-ray photoelectron spectroscopy (XPS) at the free-electron laser FERMI. Lifetimes of the chemical shifts at the S 2p edge support previous gas-phase experiments [1]. In comparison to its isomer 2-thiouracil [3], the

molecule shows an additional excited-state spectral feature.

[1] Chem. Phys. 515, 572 (2018); [2] J. Am. Chem. Soc. 140, 16087-16093 (2018); [3] Nat. Comm. 13, 198 (2022)

MO 5.6 Tue 12:15 HS XVI

Excited state dynamics of 4a,4b-Azaboraphenanthene — •JONAS FACKELMAYER, MICHAEL BÜHLER, MICHAEL MÜLLER, JAN-NIK MARKERT, and INGO FISCHER — Julius-Maximilians Universität, Würzburg, Deutschland

With growing interest in renewable energy generation, efficiently harnessing solar power has emerged as a major focus of both research and industry. The efficiency of organic solar cells might be increased significantly utilizing the photophysical process of singlet fission, a process in which a single excited singlet state splits into two triplet states therefore increasing the number of charge carriers generated from a single photon. Among the molecules that exhibit this process, polycyclic aromatic hydrocarbons (PAHs) are particularly noteworthy, as their optoelectronic properties can be tailored through the substitution of carbon units with boron and nitrogen.

In our most recent study we investigated the excited states dynamics of 4a,4b-azaboraphenanthene by picosecond time-resolved photoionization in a supersonic jet. A resonance-enhanced multi photon ionization (REMPI) spectrum reveals the S_1 origin at around 22880 cm^{-1} and shows many vibronic bands. Time-resolved time-of-flight and photoelectron imaging experiments with pump wavelengths between 401 and 437 nm and probe wavelengths of 351 and 263,5 nm yield time constants between 20 and 35 ps. The experiments are accompanied by computational studies to gain further insights into the involved vibrational modes and deactivation mechanisms.

MO 5.7 Tue 12:30 HS XVI

Ultrafast photoisomerization dynamics of protonated azobenzene in an ion trap — •MARCEL J. P. SCHMITT¹, GEREON NIEDNER-SCHATTEBURG¹, SABINE BECKER¹, CAROLIN MÜLLER², and CHRISTOPH RIEHN¹ — ¹Department of Chemistry, RPTU Kaiserslautern — ²Computer Chemistry Center, FAU Erlangen-Nürnberg, Erlangen

The E/Z photoswitchability of azobenzenes is widely used in biological, medicinal,[1] and optical applications as molecular machines[2] and reversible photoswitchable metallocycles.[3] Less is known about the photophysics and deactivation processes of simple protonated azobenzene compound. Here, we report transient photodissociation action spectra of isolated azonium monocations that reveal ultrafast dynamics of the E isomers. Multiexponential electronic decays in the sub-ps and ps time regimes occur with faster decay rates as for neutral azobenzene. Superimposed, there is a rapidly damped wave packet dynamics of 0.4 ps oscillations that indicate torsional modes of isomerization. These findings find support by nonadiabatic dynamics simulations (CASSCF) that decipher deactivation pathways.

[1] M. Medved', M. Di Donato, W. J. Buma, A. D. Laurent, L. Lameijer, T. Hrivnák, I. Romanov, S. Tran, B. L. Feringa, W. Szymanski, G. A. Woolley, J. Am. Chem. Soc. 2023, 145, 19894. [2] S. Megow, H.-L. Fitschen, F. Tuzcek, F. Temps, J. Phys. Chem. Lett. 2019, 10, 6048. [3] R. I. Petrikat, J. Hornbogen, M. J. P. Schmitt, E. Resmann, C. Wiedemann, N. I. Dilmen, H. Schneider, A. M. Pick, C. Riehn, R. Diller, S. Becker, Chem. Eur. J. 2024, 30, e202400205.

MO 5.8 Tue 12:45 HS XVI

Probing UV-induced dynamics of phenanthridine with time-resolved X-ray absorption and X-ray photoelectron spectroscopy — •DOROTHEE SCHAFFNER¹, CONSTANT SCHOUDER², KIRA DIEMER¹, XINCHENG MIAO¹, EMIL KARAEV¹, DENNIS MAYER³, AUDREY SCOGNAMIGLIO², ANDRE AL HADDAD⁴, ANTOINE SARRACINI⁴, GREGOR KNOPP⁴, LOU BARREAU², LIONEL POISSON², PATRICK HEMBERGER⁴, KIRSTEN SCHNORR⁴, ROLAND MITRIC¹, and INGO FISCHER¹ — ¹University of Würzburg, Germany — ²ISMO, Paris-Saclay University, France — ³DESY, Hamburg, Germany — ⁴PSI, Villigen, Switzerland

Modifying polycyclic aromatic hydrocarbons (PAHs) by replacing a carbon by a nitrogen atom introduces $n\pi^*$ states into the molecules, in addition to existing $\pi\pi^*$ states. This leads to an alteration in optoelectronic properties making nitrogen-containing PAHs (PANHs) promising candidates e.g. for organic photovoltaic devices. In this experiment we investigated the excited state dynamics of the PANH phenanthridine after UV excitation into the S_3 state ($\pi\pi^*$ character). Using the Maloja endstation at SwissFEL, time-resolved X-ray absorption and photoelectron spectra were recorded near the N1s edge that are par-

ticularly sensitive towards $n\pi^*$ states. Significant shifts are observed in the time-resolved spectra and time constants for the deactivation process were derived. Spectral features of the excited states and time

constants are compared to theoretical results from surface hopping dynamics simulations combined with TDDFT calculations.

MO 6: Molecular Spectroscopy of Liquid Jets II

Time: Tuesday 11:00–13:00

Location: HS XV

MO 6.1 Tue 11:00 HS XV

Determination of chemical kinetics from diffusion limited chemical reactions in free-flowing liquid flat-jets — ●HANNES CHRISTIAN SCHEWE¹, NICOLAS VELASQUEZ², BRUNO CREDIDIO², AARON GHRIST², ANDREAS OSTERWALDER³, GERARD MEIJER², BERND WINTER², and CHRISTOPHE NICOLAS⁴ — ¹J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ³Institute for Chemical Sciences and Engineering (ISIC), Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ⁴Synchrotron SOLEIL, Gif-sur-Yvette Cedex, France

We presents a methodology for conducting chemical kinetics studies at the interface between two (aqueous) solutions. When two streams from two microchannels impinge under laminar flow conditions, a flat-leaf structure forms, thereby creating an inherent liquid-liquid interface between the two solutions flowing along each other. Initially, the chemiluminescence from a luminol oxidation reaction is employed to demonstrate that the fluids do not exhibit turbulent mixing in the first leaf of a flat-jet, thus providing a clean interface between the liquids from the impinging jets [1]. Next, we examine the (de-)protonation dynamics of amine or carboxylic groups, which can be studied using either X-ray absorption spectroscopy to characterize electronic structure changes or Raman microscopy to quantify vibrational changes. We illustrate how kinetic data is obtained wherein diffusion represents the sole transport process responsible for mixing across the liquid-liquid interface. [1] H.C.Schewe et. al. J. Am. Chem. Soc. 2022, 144, 17

MO 6.2 Tue 11:15 HS XV

Electronic dynamics created at conical intersections and its dephasing in aqueous solution — ●YI-PING CHANG¹, TADAS BALCIUNAS^{1,2}, ZHONG YIN², MARIN SAPUNAR³, BRUNO TENORIO⁴, ALEXANDER PAUL⁵, SHOTA TSURU⁶, HENRIK KOCH⁵, JEAN-PIERRE WOLF¹, SONIA CORIANI⁴, and HANS JAKOB WÖRNER² — ¹Université de Geneve, Switzerland — ²ETH Zürich, Switzerland — ³Ruder Boskovic Institute, Croatia — ⁴DTU, Denmark — ⁵NTNU, Norway — ⁶Ruhr University Bochum, Germany

Understanding the electronic dynamics of molecular systems is important for many fields in photophysics and photochemistry. This is especially challenging in the vicinity of a conical intersection, where the Born-Oppenheimer approximation breaks down. In this work [1], we present two experimental breakthroughs: (1) the observation of electronic and vibrational dynamics corresponding to a circular rearrangement of the electronic structure created by conical intersection dynamics and (2) the sub-40 fs dephasing induced by aqueous solvation. Using a state-of-the-art table-top HHG source covering the entire water window, we performed time-resolved X-ray absorption spectroscopy (XAS) of single-UV-photon-excited liquid and gaseous pyrazine samples. At the carbon and nitrogen K-edges, we observed different non-adiabatic dynamics between gas and liquid phases, showing large-amplitude rearrangement of the electronic structure caused by the conical intersection and dephasing of electronic dynamics due to solvation. [1]Y.-P. Chang*, T. Balciunas*, Z. Yin*, M. Sapunar*, B.N.C. Tenorio*, A. Paul* et al. Nat. Phys. (2024).

MO 6.3 Tue 11:30 HS XV

Impact of solvation on the ultrafast ring-opening dynamics of furfural — ●JOEL TRESTER^{1,2}, PENGJU ZHANG^{1,3}, ROBIN SANTRA^{2,4,5}, LUDGER INHETER^{2,5}, and HANS JAKOB WÖRNER¹ — ¹Laboratory of Physical Chemistry, ETH Zürich, Zurich, Switzerland — ²Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China — ⁴Department of Physics, Universität Hamburg, Hamburg, Germany — ⁵Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany

We investigated the photoinduced ring-opening dynamics of furfural in

both the gas phase and pure liquid phase using a table-top monochromatized high-harmonic source combined with heatable in-vacuum sample delivery and liquid micro-jet technology. By leveraging a UV-pump XUV-probe scheme we have performed time-resolved photoelectron spectroscopy (TRPES) to access all outer-valence molecular orbitals. By achieving excellent agreement with hybrid QM/MM surface-hopping molecular dynamics simulations, this study provides the first comprehensive comparison of such dynamics between the gas and liquid phases under identical experimental conditions. Notably, we reveal that the underlying mechanism of ring opening changes significantly from the gas to the liquid phase, both in timescale and pathways. This work opens new perspectives in the field of ultrafast photochemical dynamics, by enabling a detailed exploration of solvent effects on nuclear dynamics triggered by electronic relaxation on ultrafast timescales.

MO 6.4 Tue 11:45 HS XV

Multielectron coincidence spectroscopy of solvated iodide ion — ●YUSAKU TERAOKA, DANA BLOSS, GABRIEL KLASSEN, JOHANNES VIEHMANN, ADRIAN KRONE, NIKLAS GOLCHERT, ARNO EHRESMANN, and ANDREAS HANS — Universität Kassel, Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), Heinrich-Platt-Strße 40, 34132 Kassel

Radiation effects in solvated matter are of great interest, since many aspects of them are still poorly understood and better knowledge can be beneficial for radiation protection and radiation therapy. Especially, relaxation processes between core-shell ionized solvated samples and surrounding water molecules are worth investigating. They are called interatomic/intermolecular processes that dissipate deposited energy and charge to neighboring atoms and molecules. Here, the final states of initially ionized targets can be less charged compared to the case that the target is an isolated system where Auger decay most likely occurs. For a better understanding of complex decay processes of irradiated atoms and molecules in solution, Auger cascade processes, that create highly charged final states, and its suppression via competitive interatomic/intermolecular decay processes, of core ionized iodide anion in aqueous solution was investigated. Results are obtained by a combination of liquid microjet technique and multielectron coincidence spectroscopy.

MO 6.5 Tue 12:00 HS XV

Photoelectron spectroscopy from microjets and flatjets — ●BRUNO CREDIDIO¹, DOMINIK STEMER¹, HANNES CHRISTIAN SCHEWE², SEBASTIAN MALERZ¹, MICHELE PUGINI¹, FLORIAN TRINTER¹, HENRIK HAAK¹, UWE HERGENHAIN¹, GERARD MEIJER¹, SREPHAN THÜRMER³, and BERND WINTER¹ — ¹Fritz Haber Institute of the Max Planck Society, Berlin, Germany — ²Czech Academy of Sciences, Prague, Czech Republic — ³Kyoto University, Kyoto, Japan

Among its various successful applications, LJ-PES (Liquid Jet Photoelectron Spectroscopy) enables the the study of biological molecules in their environment of relevance, i.e., aqueous phase. Despite that, the curved geometry of a LJ had hampered, e.g., soft X-ray absorption studies. This has prompted the development of planar flatjets (FJs) which has now evolved into a well-matured technique. Several experimental approaches have been realized, and their applicability to PES will be evaluated. Furthermore, the larger surface area of FJs is well suited for exploring angular-resolved scattering of a molecular beam from a planar liquid, including aqueous solution. The FJ geometry is also superior when detecting Photoelectron Angular Distributions (PADs). Our other focus here is on the unique ability to generate a flowing well-defined liquid-liquid interface in vacuum, acting as a steady-state chemical reactor and defined reaction time, accessible by IR, optical and X-ray photon detection. I will finally discuss the generation of an electric potential across the FJ that may be used to modify solution-vacuum structural and electric properties.

MO 6.6 Tue 12:15 HS XV

Time-resolved photoelectron spectroscopy of a biomimetic

photoswitch NHIP — ●OLEG KORNILOV¹, XINGJIE FU², MATTHEW MGBUKWU², ALINA KHODKO¹, JEREMIE LEONARD², and STEFAN HAACKE² — ¹Max Born Institute, Berlin, Germany — ²Institute of Physics and Chemistry of Materials, Strasbourg, France

Time-resolved photoelectron spectroscopy (TRPES) using XUV pulses from high-order harmonic generation is the state-of-the-art powerful experimental technique, which can probe transient electronic states of relaxing molecules down to their electronic ground states, follow dynamics through optically *dark* states and conical intersections. In this contribution we will report on the recent progress in studies of ultrafast isomerization of N-protonated indanylidene pyrroline Schiff bases (NHIP) using TRPES. This chromophore mimics photoisomerization properties of retinal Schiff bases in rhodopsin. We record ultrafast relaxation of the electronically excited molecule solvated in water, which appears to be nearly ballistic, and discuss the observations in comparison with the transient absorption spectroscopy results published previously. Measurements presented here open route to direct observation of ultrafast relaxation via conical intersections, which are typically not visible in all-optical time-resolved measurements.

MO 6.7 Tue 12:30 HS XV

Field Resolved Spectroscopy of flat liquid sheets — ●KILIAN SCHEFFTER^{1,2}, ANCHIT SRIVASTAVA^{1,2}, ANDREAS HERBST^{1,2}, SOYEON JUN^{1,2}, and HANIEH FATTAHI^{1,2} — ¹Max Planck Institute for the Science of Light, Erlangen, Germany — ²Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

We present femtosecond fieldoscopy at near-petahertz frequencies in flat liquid sheets. The interaction between femtosecond optical pulses and molecules in a sample results in the imprint of a molecular response on the electric field of the excitation pulses. By resolving the electric field of the transmitted pulses with attosecond precision, we achieve broadband background-free spectroscopic detection of molecules with high dynamic range and sensitivity. In liquid-phase measurements, the container's material often introduces absorption, dispersion, bire-

fringence and nonlinearity, which limits the detection sensitivity. To overcome these challenges, we developed a 3D printed nozzle capable of producing micrometer thick liquid sheets, enabling direct spectroscopic measurements of liquids. This talk will present the integration of the liquid jet into field-resolved spectroscopy, allowing for the measurement of Raman, overtone, and combination bands of liquid samples across the entire fingerprint region.

MO 6.8 Tue 12:45 HS XV

Liquid sample delivery at EuXFEL — ●JOANA VALERIO, MARCO KLOOS, KATERINA DÖRNER, HUIJONG HAN, ELISA DELMAS, AGNIESZKA WRONA, GISEL PEÑA, ALEXANDER GIERKE, ELIZABETH GALTRY, and JOACHIM SCHULZ — European XFEL, Schenefeld, Germany

One of the most distinctive characteristics of the European XFEL is the high repetition rate of the X-ray pulses. The intra-train repetition rate of up to 4.5 MHz represents a significant challenge for the sample injection systems. The Sample Environment & Characterisation (SEC) group of the EuXFEL is developing sample delivery systems for all scientific instruments, in addition to providing user support in sample preparation, characterization, and delivery.

Cylindrical microjet injection systems remain the most prevalent type of sample injection system employed in the fields of soft and hard X-ray science. Nevertheless, this methodology is subject to several intrinsic constraints. For example, the curved surface of the nozzle presents a challenge in determining the path length of the X-rays within the sample. The sample must have a well-defined and controllable thickness of just a few tens of microns or less, and the efficiency of sample usage requires the use of micron-sized liquid sheet jets. In light of these limitations, various 3D-printed nozzle designs have been developed to produce micron-thick and highly stable microscopic flat sheet jets. These designs are based on colliding and impingement nozzle designs, to make this technology more widely available to users, especially for spectroscopy.

MO 7: Attosecond Physics I (joint session A/MO)

Time: Tuesday 11:00–12:30

Location: GrHS Mathe

Invited Talk

MO 7.1 Tue 11:00 GrHS Mathe

Water Window HHG continua driven by sub-cycle, nonsinusoidal IR Pulses — ●FABIAN SCHEIBA^{1,2,3}, MIGUEL SILVA^{1,2}, GIULIO MARIA ROSSI^{1,3}, ROLAND E. MAINZ^{1,2,3}, MAXIMILIAN KUBULLEK^{1,2}, RAFAEL D. Q. GARCIA^{1,2}, and FRANZ X. KÄRTNER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL and Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ²Physics Department, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — ³The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We present the next milestone of our infrared (IR) Parametric Waveform Synthesizer (PWS), that is the generation of HHG continua in the Water Window (WW) spectral region, up to 450 eV. The IR driver pulses are characterized to a pulse duration of 2.8 fs at 1.6 μm central wavelength and an update of the attosecond beamline apparatus enables for high pressure phase matching in Helium and Neon gases. The PWS allows for sub-cycle control of the HHG process and following control of the HHG spectra. Scans of the given phase parameters of the driving electric field show a strong dependence of the generated HHG and therefore unmatched tuning capabilities. Furthermore, calibrated measurements of the HHG yield allows us to claim a significant efficiency increase compared to a few cycle sinusoidal driver pulse.

MO 7.2 Tue 11:30 GrHS Mathe

Towards AI-enhanced online-characterization of ultrashort X-ray free-electron laser pulses — ●THORSTEN OTTO^{1,2,4}, KRISTINA DINGEL², LARS FUNKE³, SARA SAVIO^{3,4}, LASSE WÜLFING^{3,4}, BERNHARD SICK², WOLFRAM HELML³, and MARKUS ILCHEN^{1,4} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ²University of Kassel, Intelligent Embedded Systems, Wilhelmshöher Allee 73, 34121 Kassel, Germany — ³Technische Universität Dortmund, Fakultät für Physik, Maria-Göppert-Mayer-Straße, 44227 Dortmund, Germany — ⁴Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149 22761 Hamburg

X-ray free-electron lasers provide ultrashort X-ray pulses with durations typically in the order of femtoseconds, but recently even entering the attosecond regime. The technological evolution of XFELs towards well-controllable light sources for precise metrology of ultrafast processes can only be achieved using new diagnostic capabilities for characterizing X-ray pulses at the attosecond frontier. The spectroscopic technique of photoelectron angular streaking has successfully proven how to non-destructively retrieve the exact time-energy structure of XFEL pulses on a single-shot basis. By using deep learning algorithms, we show how this technique can be leveraged from its proof-of-principle stage towards routine diagnostics at XFELs providing precise feedback in real time.

MO 7.3 Tue 11:45 GrHS Mathe

Extracting RABBIT-like phase information from time dependent transient absorption spectra — ●JULIAN JAKOB¹, CORNELIA BAUER¹, MURAT-JAKUB ILHAN¹, DIVYA BARTHI², CHRISTIAN OTT², THOMAS PFEIFER², KLAUS BARTSCHAT³, and ANNE HARTH¹ — ¹Center for Optical Technologies, Aalen University, Aalen, Germany — ²Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany — ³Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA

We investigate transient absorption spectroscopy by exploring how the spectral phase of the attosecond pulse train modulates the optical density signal. The process is driven by the interaction of extreme ultraviolet (XUV) and near-infrared (NIR) fields, with their relative time delay playing a crucial role in shaping the dynamics [1]. As demonstrated in Reconstruction of Attosecond Beating by Interference of Two-Photon Transitions (RABBIT) experiments, the XUV phase can be measured by examining the photoionization electron spectrum as a function of the time delay between the XUV and NIR fields [2]. Similarly, the spectral phase of the XUV field imprints itself in oscillations of the optical density, which occur at twice the NIR frequency ($2\omega_{\text{NIR}}$). Using a few-level model, we simulate the quantum dynamics and validate our findings by solving the time-dependent Schrödinger equation (TDSE)

for atomic hydrogen. This approach reveals how the spectral phase modulates the optical density, thereby providing a direct link to the underlying attosecond electron dynamics. [1] Holler, Phys. Rev. Lett. 106, 123601 (2011), [2] Hentschel, Nature 414, 509-513 (2001)

MO 7.4 Tue 12:00 GrHS Mathe

In silico approach for understanding experimental sub-cycle driven high harmonic generation from XUV to soft X-rays.

— ●RAFAEL DE Q. GARCIA^{1,2}, MAXIMILIAN KUBULLEK^{1,2}, MIGUEL SILVA^{1,2}, ROLAND E. MAINZ^{1,2,3}, FABIAN SCHEIBA^{1,2,3}, GIULIO M. ROSSI^{1,3}, and FRANZ X. KÄRTNER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL and Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ²Physics Department, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — ³The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

High harmonic generation (HHG) has since long been used for generating tabletop XUV to soft X-ray isolated attosecond pulses used for ultrafast science. However, as the pulses driving HHG get shorter, achieving even sub-cycle duration, new challenges are faced both experimentally and theoretically to understand which electric field is producing HHG and how phase-matching of HHG actually happens in a medium. To answer these questions, we combine an in situ pulse characterization technique with a 1D optical and HHG-field propaga-

tion code. With these two tools, we simulate the outcomes of an experiment performed with our parametric waveform synthesizer, which drives HHG with either few-cycle or synthesized sub-cycle pulses, under different macroscopic conditions. It is shown, that this method enables qualitative and quantitative agreement between experiment and simulation, answering fundamental questions about sub-cycle driven HHG such as efficiency increase and plasma propagation effects.

MO 7.5 Tue 12:15 GrHS Mathe

The Quantum Superluminality of Tunnel-ionization — ●OSSAMA KULLIE — University of Kassel, Institute of Physics

In our tunnel-ionization model presented in previous work[1,2,3,4], we showed that adiabatic and nonadiabatic tunnel-ionization time amounts to determine the barrier time-delay with good agreement with the attoclock measurement and that it corresponds to the dwell time and the interaction time. In the present work, we show that the barrier time-delay for H-like atoms with large nuclear charge can be superluminal (quantum superluminality), which can be validated experimentally using the attoclock scheme. We discuss the quantum superluminality for the different experimental calibrations of the attoclock. [1] O. Kullie, submitted to J. Phys. Comm. (2024). [2] Ossama Kullie and Igor Ivanov, Ann. of Phys 464, 169648 (2024). [3] O. Kullie, Phys. Rev. A 92, 052118 (2015). [4] O. Kullie. J. Phys. Commun. 2 065001 (2018).

MO 8: Strong-Field and Ultrafast Phenomena (joint session Q/MO)

Time: Tuesday 11:00–12:45

Location: HS V

Invited Talk

MO 8.1 Tue 11:00 HS V

Strong-field physics and nonlinear optical phenomena in two-dimensional honeycomb materials — ●ANNA GALLER — Institute of Theoretical and Computational Physics, TU Graz, Austria

Strong-field physics and extreme nonlinear optical processes in solids have emerged as powerful tools for ultrafast spectroscopy of electron dynamics. Ultrashort intense laser pulses have also been used to control and probe the valley pseudospin in two-dimensional honeycomb materials like transition-metal dichalcogenides. These phenomena are governed by the material-specific electronic structure and the nature of light-matter interaction. In this talk, I will present how ab-initio calculations can provide insights into these processes. Specifically, I will explore the role of the Floquet light-driven electronic structure in nonlinear optical phenomena and demonstrate how valley polarization and photocurrents in monolayer hexagonal boron nitride can be controlled using elliptically polarized, ultrashort laser pulses. Additionally, I will address high-harmonic generation (HHG) in two-dimensional materials, focusing on how interference effects from HHG emissions at distinct k-points in the Brillouin zone explain spectral features like peak splitting in monolayer WS₂. Finally, I will compare these simulation results with experimental observations to highlight the predictive power of our theoretical approach.

MO 8.2 Tue 11:30 HS V

What does extreme nonlinear optics tell about black holes? — ●LORENZO M. PROCOPIO^{1,2}, RAUL AGUERO-SANTACRUZ³, DAVID BERMUDEZ³, and LORENZO PROCOPIO² — ¹Department of Physics, Paderborn University, Warburger Str. 100, 33098 Paderborn, Germany — ²Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 761001, Israel — ³Department of Physics, Cinvestav, A.P. 14-740, 07000 Ciudad de Mexico, Mexico

In 1974, Hawking predicted that black holes should emit radiation. Seven years later, Unruh showed a mathematical analogy of the Hawking effect with sound waves in a fluid flow. Since then, several systems have emerged to demonstrate experimentally Hawking's predictions. Extreme nonlinear optics is a promising platform to study analog event horizons in photonic crystal fibers, where the event horizon is created with near-single-cycle light pulses. We experimentally studied the backreaction of Hawking radiation and present a more complete description of the Hawking process in fiber-optical analogues. For astrophysical black holes, this process would correspond to the mechanism of how Hawking radiation is made at the event horizon, how quanta of gravity produce quanta of radiation. In astrophysics, such a process is elusive and unknown, in extreme nonlinear fiber optics we believe to have observed it.

MO 8.3 Tue 11:45 HS V

Photocurrent control in a light-dressed Floquet topological insulator — ●WEIZHE LI¹, DANIEL LESKO¹, TOBIAS WEITZ¹, SIMON WITTIGSCHLAGER¹, CHRISTIAN HEIDE^{1,2}, OFER NEUFELD³, and PETER HOMMELHOFF^{1,4} — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — ²Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — ³Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel — ⁴Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Light-dressed materials, based on Floquet engineering, offers unique opportunities to design transient band structures. Most commonly, circularly-polarized dressing light can generate topologically non-trivial nonequilibrium states known as Floquet topological insulators (FTIs) which host a variety of topological phenomena. Floquet engineering with strong optical fields opens routes to optically tunable band structures and devices for petahertz electronics.

Here we demonstrate coherent control of photocurrents in light-dressed graphene. Circularly-polarized laser pulses dress the graphene into an FTI, and phase-locked second harmonic pulses drive electrons in the FTI. We map the resulting dynamics onto two-color phase dependent photocurrents. This approach allows us to measure all-optical anomalous Hall currents and photocurrent circular dichroism. Furthermore, we map out the attosecond Floquet phase by varying the two-color phase. The coherent control of photocurrents in graphene-based FTI connects optics tools to condensed matter physics.

MO 8.4 Tue 12:00 HS V

Strong-field electron dynamics in non-classical light after photoemission from nanometric needle tips — ●JONATHAN PÖLLOTH¹, JONAS HEIMERL¹, ANDREI RASPUTNYI², STEFAN MEIER¹, MARIA CHEKHOVA^{1,2}, and PETER HOMMELHOFF^{1,2,3} — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — ²Max-Planck-Institut für die Physik des Lichts (MPL), 91058 Erlangen — ³Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

In the past, strong-field physics and quantum optics were two seemingly unrelated fields of research. However, in recent years, the development of intense non-classical light sources such as bright squeezed vacuum (BSV) has made it possible to connect these topics and to explore nonlinear interaction processes between intense quantum light and matter. Recent theoretical [1] and experimental [2] studies investigate the influence of the quantum state of light on strong-field processes such as high harmonic generation. For the case of nonlinear electron photoemission from needle tips, it was shown that the elec-

trons inherit the number statistics of the driving light state [3]. Here, we will present the first measurements of strong-field electron energy spectra for photoemission from nanometric needle tips driven by BSV and explain them based on the theoretical frameworks.

[1] A. Gorlach *et al.*, *Nat. Phys.* **19**, 1689-1696 (2023)

[2] A. Rasputnyi *et al.*, *Nat. Phys.* (2024)

[3] J. Heimerl *et al.*, *Nat. Phys.* **20**, 945-950 (2024)

MO 8.5 Tue 12:15 HS V

Ultrafast photoemission from gold tips in the intermediate regime — ●LEON BRÜCKNER¹, JONAS HEIMERL¹, STEFAN MEIER¹, PHILIP DIENSTBIER¹, CONSTANTIN NAUK^{1,2}, and PETER HOMMELHOFF^{1,3} — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — ²Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — ³Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

The intermediate regime in photoemission, corresponding to a Keldysh parameter γ around 1-3, lies in between the extreme cases of multiphoton and the quasi-static tunneling emission. This regime shows characteristic features, namely a smooth decrease in the nonlinearity of the emission process as well as the appearance of channel closings. In strong-field experiments at sharp metal needle tips, this picture becomes more complex due to the possible influence of space-charge effects arising from the large number of emitted electrons. We investigate the emitted current from an array of sharp gold tips illuminated with 25 fs laser pulses. Through comparison with time-dependent Schrödinger equation (TDSE) calculations, we identify characteristic

intensity-dependent changes in the rate scaling and discuss the influence of space-charge effects.

MO 8.6 Tue 12:30 HS V

Recent advances in splitting and coherent beam recombining of femtosecond beams/pulses using optical vortex lattices — ●LYUBOMIR STOYANOV¹, YINYU ZHANG^{2,3}, ALEXANDER DREISCHUH¹, and GERHARD PAULUS^{2,3} — ¹Department of Quantum electronics, Faculty of Physics, Sofia University — ²Institute of Optics and Quantum Electronics, Friedrich Schiller University Jena — ³Helmholtz Institute Jena

In this work, we will present our recent advances in addressing spectral broadening and temporal compression of high-energy femtosecond pulses by the controllable splitting and coherent beam recombining of such beams/pulses using optical vortex lattices. This controllable and reversible beam reshaping technique known from singular optics is the key feature in this approach. Using fused silica vortex phase plates, etched with square-shaped optical vortex lattices we achieved an experimental realization of controllable beam splitting of intense femtosecond beams/pulses, followed by nonlinear spectral broadening (both in ambient air and fused silica substrate) and a final coherent beam recombination. Moreover, the compression in time of the spectrally broadened pulses down to the Fourier transform limit is demonstrated as well. In our view, the results confirm the feasibility of the proposed idea and provide strong motivation for further optimization and investigation serving as potential alternative to the established methods for coherent beam recombining.

MO 9: Poster – Novel Approaches

Time: Tuesday 14:00–16:00

Location: Tent

MO 9.1 Tue 14:00 Tent

Spectroelectrochemical cell designs for ultrafast spectroscopy — ●REBECCA FRÖHLICH and TOBIAS BRIXNER — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Charged molecules play essential roles in many photophysical and photochemical processes. Therefore, the identification of chemical redox species and the kinetic evolution of their photoexcited states is highly desirable. However, unequivocal identification of species remains challenging when reaction intermediates are chemically unstable and the dynamics take place on an ultrafast timescale. The ultrafast dynamics of specific redox species can be accessed by combining electrochemical methods with transient absorption spectroscopy [1,2]. Here, we present and compare several spectroelectrochemical cells of our own design for application in time-resolved spectroelectrochemistry. The cell designs feature flow options as well as optically transparent thin-layer geometries with the aim of realizing a simple setup and reliable performance. The advantages and drawbacks of each cell design are illustrated by performing cyclic voltammetry, absorption spectroelectrochemistry, and ultrafast transient absorption spectroscopy experiments.

[1] S. Bold *et al.*, *Chem. Commun.* **54**, 10594 (2018).

[2] R. Fröhlich *et al.*, *J. Chem. Phys.* **160**, 234201 (2024).

MO 9.2 Tue 14:00 Tent

Optimized Velocity Map Imaging Spectrometer for Deep-UV Measurements — ●FABIAN WESTMEIER, NICOLAS LADDA, JOCHEN MIKOSCH, THOMAS BAUMERT, and ARNE SENFTLEBEN — Institute of Physics and CINSaT, University of Kassel, 34132 Kassel, Germany

Velocity Map Imaging spectroscopy [1] is a powerful method for investigating photoionization processes, by projecting the photoelectron angular distribution onto a position-sensitive detector. We present a spectrometer that is used to study the dynamics of chiral molecules via time-resolved photoelectron circular dichroism [2] with deep-UV photons. Such experiments often experience a high level of background signals due to photoelectrons generated at the spectrometer electrodes from scattered photons. Here we present our successful approaches to reduce this background. We achieved the biggest improvement by using thin electrodes, which minimize the surface area exposed to scattered light. A large hole in the repeller plate combined with an additional high-voltage electrode underneath results in the photoelectrons

emitted from the repeller plate being captured by the electrode above. Furthermore, we designed light baffles exhibiting high UV absorption [3], which confine the opening angle for scattered light. To minimize overall scattering, we used thin single-crystal calcium fluoride (CaF₂) windows.

[1]: A. T. J. B. Eppink, D. H. Parker, *Rev. Sci. Instrum.* **68**, 3477-3484 (1997)

[2]: C. Lux *et al.*, *Angew. Chem. Int. Ed.* **51**, 5001-5005 (2012)

[3]: O. J. Clarkin, Dissertation, Queen's University, Canada (2012)

MO 9.3 Tue 14:00 Tent

Generalized energy gap law: An open system dynamics approach to non-adiabatic phenomena in molecules

— ●NICO BASSLER^{1,2}, MICHAEL REITZ³, RAPHAEL HOLZINGER⁴, AGNES VIBÓK^{5,6}, GÁBOR HALÁSZ⁷, BURAK GURLEK⁸, and CLAUDIU GENES^{1,2} — ¹Max Planck Institute for the Science of Light, D-91058 Erlangen, Germany — ²Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), D-91058 Erlangen, Germany — ³Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, California 92093, USA — ⁴Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria — ⁵Department of Theoretical Physics, University of Debrecen, H-4002 Debrecen, Hungary — ⁶ELI-ALPS, ELI-HU Non-Profit Ltd, H-6720 Szeged, Hungary — ⁷Department of Information Technology, University of Debrecen, H-4002 Debrecen, Hungary — ⁸Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany

Non-adiabatic phenomena, resulting from the breakdown of the Born-Oppenheimer approximation, influence most photo-physical and photo-chemical processes, limiting molecular quantum efficiency. The energy gap law, established five decades ago, predicts non-radiative decay with an exponential dependence on the energy gap. Here, we revisit and extend this theory to incorporate vibrational relaxation, dephasing, and radiative loss with a focus on the structure of the nonadiabatic coupling.

MO 9.4 Tue 14:00 Tent

Generation of broad-bandwidth deep ultraviolet pulses with achromatic second harmonic generation — ●NILS-OLIVER SCHÜTZ, LUKAS BRUDER, FERDINAND BERGMEIER, and ULRICH BANGERT — University of Freiburg, Institute of Physics, 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 ($> 100\text{kHz}$) 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]. First results will be presented.

MO 9.5 Tue 14:00 Tent

High-repetition-rate ultrafast electron diffraction with direct electron detection — FERNANDO RODRIGUEZ DIAZ, ANDREY RYABOV, MARK MERO, and •KASRA AMINI — Max-Born-Institut,

Max-Born-Straße 2A, 12489, Berlin, Germany

We present a novel ultrafast electron diffraction (UED) instrument that operates at high repetition rates and utilizes direct electron detection, enabling the measurement of time-resolved electron scattering signals with single-electron pulses at 30 kHz. With this state-of-the-art setup, we achieved time-resolved measurements from thin-film solid samples, demonstrating a difference contrast signal, $\Delta I/I_0$, as low as 10^{-5} and an instrument response function of 184 fs (FWHM) without temporal compression and a 1-metre cathode-sample distance. This significant advancement, combined with ongoing developments in RF-compressed and THz-streaked electron pulses, lays the groundwork for investigating ultrafast photochemical reaction dynamics in gas-phase molecules with sub-100-fs total temporal resolution.

MO 10: Poster – Chirality

Time: Tuesday 14:00–16:00

Location: Tent

MO 10.1 Tue 14:00 Tent

Investigation of chiral structural dynamics using time-resolved PECD — •NICOLAS LADDA, FABIAN WESTMEIER, TONIO ROSEN, SUDHEENDRAN VASUDEVAN, SIMON RANECKY, SAGNIK DAS, TILL JAKOB STEHLING, KRISCHNA KANT SINGH, HENDRIKE BRAUN, JOCHEN MIKOSCH, THOMAS BAUMER, and ARNE SENFTLEBEN — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The dynamic change of the chiral character during laser-induced vibrational motion in an electronically excited state of methyl p-tolyl sulfoxide (MTSO) is investigated [1]. For this purpose, we measure the forward/backward asymmetry of the photoelectron angular distribution (PAD) with respect to the propagation direction of ionising circularly polarised light of the randomly oriented chiral molecule, known as photoelectron circular dichroism (PECD) [2]. The vibrational motion in the electronically excited state changes the chiral character of the molecule, which can be investigated by studying the time-resolved PECD with UV femtosecond laser pulses. For this purpose, a two-colour pump-probe setup consisting of 262 nm and 197 nm is used. The current state of the experiment will be reported.

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

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

MO 10.2 Tue 14:00 Tent

Towards the measurement of Photoelectron Circular Dichroism of (M)-[4] triangulane — •TONIO ROSEN, NICOLAS LADDA, SIMON RANECKY, SAGNIK DAS, SUDHEENDRAN VASUDEVAN, TILL STEHLING, FABIAN WESTMEIER, JOCHEN MIKOSCH, KRISHNA SINGH, HENDRIKE BRAUN, ARNE SENFTLEBEN, 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 its highest occupied molecular orbital [1]. 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 [2]. 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. [1] A. de Meijere et al., *The First Enantiomerically Pure [n]Triangulanes and Analogues: σ -[n]Helicenes with Remarkable Features*. *Chem. Eur. J.* 8. [2] C. Lux et al., *Circular dichroism in the photoelectron angular*

distributions of camphor and fenchone from multiphoton ionization with femtosecond laser pulses. *Angew. Chem. Int. Ed.* 51.

MO 10.3 Tue 14:00 Tent

Coherent control of circular dichroism in ion yield of chiral molecules — •SAGNIK DAS, SUDHEENDRAN VASUDEVAN, NICOLAS LADDA, SIMON RANECKY, TONIO ROSEN, TILL JAKOB STEHLING, FABIAN WESTMEIER, KRISHNA KANT SINGH, ARNE SENFTLEBEN, JOCHEN MIKOSCH, THOMAS BAUMERT, and HENDRIKE BRAUN — Institut für Physik, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The use of shaped femtosecond laser pulses is a proven strategy for directing reaction and excitation pathways in molecular systems [1,2]. We have employed shaped femtosecond UV pulses to control the Circular Dichroism in Ion Yield (CDIY) of 3-methylcyclopentanone [3]. Our findings suggest that pulse duration, linear chirp, and central wavelength of the excitation can control the CDIY. Additionally, the conformation dynamics of the molecule in the excited state may contribute to enhanced CDIY. Currently, we are investigating the control of CDIY in substituted fenchone with pulse parameters similar to those above at visible wavelengths. We aim to extend our control over CDIY by exploiting more flexible and customized pulse shapes through advanced pulse shaping techniques.

[1] A. Assion et al., *Science* 282, 919-922 (1998)

[2] M. Wollenhaupt & T. Baumert, *Faraday Discuss.* 153, 9-26 (2011)

[3] S. Das et al., manuscript to be submitted (2024)

MO 10.4 Tue 14:00 Tent

Towards probing Rydberg wave packet dynamics in chiral molecules via time dependant photoelectron circular dichroism — •SAGNIK DAS, TONIO ROSEN, NICOLAS LADDA, SUDHEENDRAN VASUDEVAN, SIMON RANECKY, TILL STEHLING, FABIAN WESTMEIER, JOCHEN MIKOSCH, KRISHNA SINGH, HENDRIKE BRAUN, ARNE SENFTLEBEN, and THOMAS BAUMERT — Universität Kassel

A Rydberg wave packet is a superposition of multiple, highly excited electronic states (Rydberg states). The evolution of these wave packets exhibits radially oscillating charge density with fixed revival times [1]. These radial charge density oscillations could prove chiral sensitive in a chiral molecular potential. This Project aims to probe the Rydberg wave packet dynamics in the chiral molecules fenchone and thiofenchone using time-dependent photoelectron circular dichroism (PECD). PECD is defined as the forward-backward asymmetry in photoelectron distribution with respect to the laser propagation direction in chiral molecules ionized with circularly polarized light [2]. In this contribution, we will provide preliminary data and report on the project's current status. [1] Fielding, H. H., *Ann. Rev. Phys. Chem.*, 56, 91-117 (2005) [2] Lux, C. et al., *Angew. Chem. Int. Ed.* 51, 5001*5005 (2012)

MO 11: Poster – Polaritonic Effects in Molecular Systems (joint session MO/Q)

Time: Tuesday 14:00–16:00

Location: Tent

MO 11.1 Tue 14:00 Tent

Modifying the electronic properties of the topological systems with cavity — ●SABER ROSTAMZADEH, REMI AVRILLER, CLEMENT DUTREIX, and FABIO PISTOLESI — Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux, France

Topological systems exhibit fascinating electronic applications due to their distinctive edge and zero-mode states. A central question is how these states interact with various environments, such as intense light. Similarly, hybrid quantum systems containing a few electrons, such as quantum dots, serve as valuable models for engineering topological electronic states. These systems have also garnered significant interest in cavity quantum electrodynamics (cavity QED) for their potential to achieve ultrastrong light-matter interactions. Their simplified architectures offer significant enhancements and optimizations in electron-photon coupling. In this study, we investigate modifications in electronic transport within single and double quantum dot arrays placed inside a cavity.

MO 11.2 Tue 14:00 Tent

Vibrational dynamics of individual oscillators under Vibrational Strong Coupling — ●HELENA POULOSE¹, MATHIS NOELL², YANNIK PFEIFER¹, TILL STENSITZKI¹, CARSTEN HENKEL², WOUTER KOOPMAN², and HENRIKE MÜLLER-WERKMEISTER¹ — ¹Institut für Chemie, Universität Potsdam, Germany — ²Institut für Physik und Astronomie, Universität Potsdam, Germany

The novel field of polariton chemistry opens up a way to tune material properties and steer chemical reactions by manipulating quantum light-matter interactions. Fabry-Perot cavities can be constructed to confine electromagnetic field, allowing the light mode to strongly couple with vibrational transitions of molecules, generating quasi light-matter states, characterised by vacuum rabi splitting. However the underlying mechanism behind how it effects the reaction dynamics is not completely understood. Combining Ultrafast nonlinear spectroscopy with Strong coupling could provide insights to how the energy distribution changes when these delocalized hybrid states are formed. Experiments of vibrational dynamics can possibly provide valuable insights into the fundamental mechanisms of polaritons and how polaritons might modulate Chemistry. Here we report on our a) cavity design and characterisation, b) static polariton spectra supported by theory and c) first attempts in performing nonlinear IR and 2DIR spectra of organic compounds, like Benzaldehyde(C=O), under VSC in cavities. We aim to investigate vibrational lifetimes and energy transfer processes and examining how these depend on cavity and molecular properties.

MO 11.3 Tue 14:00 Tent

Coherent state switching using vibrational polaritons in an asymmetric double-well potential — ●LOÏSE ATTAL¹, FLORENT CALVO², CYRIL FALVO^{1,2}, and PASCAL PARNEIX² — ¹Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405 Orsay, France — ²Université Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France

The quantum dynamics of vibrational polaritonic states arising from the interaction of a bistable molecule with the quantized mode of a Fabry-Perot microcavity is investigated using {a generic} asymmetric double-well potential as a simplified one-dimensional model of a reactive molecule. After discussing the role of the light-matter coupling strength in the emergence of avoided crossings between polaritonic states, we investigate the possibility of using these crossings to trigger a dynamical switching of these states from one potential well to the other. Two schemes are proposed to achieve this coherent state switching, either by preparing the molecule in an appropriate vibrational excited state before inserting it into the cavity, or by applying a short laser pulse inside the cavity to obtain a coherent superposition of polaritonic states. The respective influences of the dipole amplitude

and potential asymmetry on the coherent switching process are also discussed.

MO 11.4 Tue 14:00 Tent

Chemical reaction rate of molecules in a cavity — ●YANNIC JOSHUA BANTHIEN¹, ABRAHAM NITZAN², and MICHAEL THORWART¹ — ¹I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany — ²Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

We determine the reaction dynamics of N identical molecular systems, each represented by a particle in a double-well potential and each coupled to the same broadened mode of an optical cavity. Every reaction system is restricted to its lowest four energy eigenstates of the double well, forming a doublet-doublet system. A Markovian approximated master equation is set up following the Feynman-Vernon approach. It is constructed for the purpose of strong system-bath interaction. We solve for the time evolution of the quantum many-body system and extract the inter- and intra-well relaxation rates, leading to the chemical reaction rate. We study the impact of the common cavity mode on the reaction rate, determine the condition under which a Rabi splitting is found, and reveal emerging cooperative effects in the transfer rate.

MO 11.5 Tue 14:00 Tent

Modifying Photoacids under Vibrational Strong Coupling — ●SWATHI SWAMINATHAN¹, JULIA BERGER², GREGOR JUNG², and THOMAS EBBESEN¹ — ¹University of Strasbourg, Strasbourg, France — ²Saarland University, Saarbrücken, Germany

Vibrational strong coupling (VSC) between molecular transitions and cavity modes can significantly alter molecular properties and intermolecular interactions in the ground state. Here we explore the properties of photoacids,^[1] which exhibit acidity in the excited state, and provide an ideal platform to explore the effects of VSC on their photo-physics. Photoacids typically exhibit characteristic fluorescence properties associated with the proton transfer from the solute to the solvent. Under cooperative VSC, we observe that this behavior is modified. This study shows that VSC can also affect excited-state properties, opening new avenues for understanding and controlling light-induced processes in molecular systems under strong coupling conditions.

[1] B. Finkler et al., Photochem. Photobiol. Sci. 2016, 15, 1544.

MO 11.6 Tue 14:00 Tent

Vibrational strong coupling: a detailed analysis of the cavity tilt angle — ●MATHIS NOELL¹, HELENA POULOSE², YANNIK PFEIFER², TILL STENSITZKI², WOUTER KOOPMAN¹, HENRIKE MÜLLER-WERKMEISTER², and CARSTEN HENKEL¹ — ¹Universität Potsdam, Institut für Physik und Astronomie — ²Universität Potsdam, Institut für Chemie

Plasmonic chemistry is an emerging field that seeks to uncover new pathways for chemical reactions. One intriguing phenomenon in this domain is the strong coupling between a plasmonic cavity field and molecular excitations, resulting in the formation of hybrid polariton states. These hybrid states can modify potential energy surfaces and potentially tune material properties to benefit from enhanced reaction rates. To deepen our understanding of polariton dynamics, we investigate an analogous system where molecular vibrational resonances hybridize with an IR Fabry-Pérot cavity field mode. In this work, we present a detailed analysis of vibrational cavity strong coupling under angular variation, including the shift in polariton energy as the cavity is tilted. Additionally, we explore the polariton composition (Hopfield coefficients) and predict transmission, reflection, and absorption spectra. Our goal is to compare these theoretical results with pump-probe experiments, thereby contributing to a more comprehensive understanding of strong coupling dynamics.

MO 12: Poster – Cold Atoms and Molecules, Matter Waves (joint session Q/A/MO)

Time: Tuesday 14:00–16:00

Location: Tent

MO 12.1 Tue 14:00 Tent

Dephasing of Rydberg excitations in optical traps — ●SIMON SCHROERS¹, LUKAS AHHLEIT¹, DANIL SVIRSKIY¹, NINA STIESDAL¹, JAN DE HAAN¹, CHRIS NILL², IGOR LESANOVSKY², WOLFGANG ALT¹, and SEBASTIAN HOFFERBERTH¹ — ¹Institut für Angewandte Physik, Universität Bonn — ²Institut für Theoretische Physik, Universität Tübingen

Collective Rydberg-excitations of N atoms by a single photon offer a distinct platform for strong light-matter interaction, due to the enhanced coupling by \sqrt{N} . This allows for instance the creation of Rydberg superatoms, namely an atom cloud smaller than the Rydberg-blockade-volume acting as an effective two level-system strongly coupled to a few-photon driving field.

On this poster we show recent experimental results of how we implement a so-called magic wavelength trap for ground state and Rydberg atoms. The magic trap equalizes the AC Stark shifts for both states, thereby enhancing the ground-to-Rydberg state coherence time. Using photon-storage measurements we demonstrate that the optimal wavelength for such a trap depends on the trap's geometry, as the almost-free Rydberg electron samples different regions of the trap.

We also show an investigation of Rabi oscillation dephasing between the ground and a collectively excited state of a superatom. Comparing simulations and experimental data we demonstrate that the frequency noise of the excitation lasers plays a significant role in the dephasing and identify the noise regimes that are most crucial for such dephasing.

MO 12.2 Tue 14:00 Tent

Chiral Van der Waals interactions between Rydberg atoms — ●FABIAN SPALLEK¹, STEFAN AULL¹, STEFFEN M. GIESSEN², KILIAN SINGER¹, ROBERT BERGER², AKBAR SALAM³, and STEFAN YOSHI BUHMANN¹ — ¹University Kassel, Germany — ²Phillips-University Marburg, Germany — ³Wake Forest University, USA

We study the Van der Waals potential between two atoms prepared in chiral superpositions of electronic Rydberg states. By harnessing external electric and magnetic fields, one can induce chiral asymmetry in the Rydberg states, which in turn gives rise to a chiral component in the near-field Van der Waals potential. This chiral component emerges from the interplay of electric and magnetic dipole-dipole interactions and contributes to the overall Van der Waals potential in addition to the conventional electric dispersion interaction. We derive effective potentials by performing various orientational averages and identify specific chiral Rydberg states that significantly enhance chiral the discriminatory component. These states offer a promising platform for realizing strong chiral interactions between Rydberg atoms, potentially enabling novel applications in quantum control and sensing.

MO 12.3 Tue 14:00 Tent

Machine learning optimized time-averaged potentials — ●MAX SCHLÖSINGER¹, OLIVER ANTON¹, VICTORIA HENDERSON^{1,3}, ELISA DA ROS¹, MUSTAFA GÜNDOĞAN¹, SIMON KANTHAK¹, and MARKUS KRUTZIK^{1,2} — ¹Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin, Germany — ²Ferdinand-Braun-Institut (FBH), Gustav-Kirchhoff-Straße 4, 12489 Berlin — ³now: RAL Space, Fermi Ave, Harwell, Didcot OX11 0QX, United Kingdom

Time-averaged potentials (TAPs) are a versatile tool for the generation and manipulation of ultracold atom clouds. Using a CCD-based setup to characterize a 2D acousto-optic deflector (2D-AOD) system, we implement and test machine learning routines to optimize 2D geometries, such as harmonic potentials. This approach allows us to compare different methods, evaluate metrics like homogeneity, and improve the predictability of the resulting potentials.

By employing optimization algorithms such as CMA-ES and various Bayesian optimizers, we compare their performance in terms of speed and efficiency. Additionally, we plan to implement an active learning optimizer to minimize the number of required iterations, which is crucial for future integration into a ⁸⁷Rb Bose-Einstein condensate (BEC) experiment. Ultimately, these advancements will enhance the evaporative cooling routine and improve the performance of a ⁸⁷Rb BEC-based quantum memory [1].

[1] Phys. Rev. Research **5**, 033003 (2023)

MO 12.4 Tue 14:00 Tent

Rydberg superatoms coupled with super-extended evanescent field nanofiber at the single-photon level — ●LUDWIG MÜLLER¹, KNUT DOMKE¹, TANGI LEGRAND¹, THOMAS HOINKES², XIN WANG¹, EDUARDO URUÑUELA¹, WOLFGANG ALT¹, and SEBASTIAN HOFFERBERTH¹ — ¹Institute of Applied Physics, University of Bonn, Germany — ²Department of Physics, Humboldt University of Berlin, Germany

Both Rydberg superatoms driven by free-space photonic modes and single emitters coupled to photonic waveguides have paved the way for strong coherent light-matter coupling at the few-photon level. By combining advantages of both ideas, we aim to achieve homogeneous coupling of multiple Rydberg superatoms coupled to a field confined by a nanofiber. Fibers with diameters of a few hundred nanometers are successfully used to trap and couple arrays of single atoms by their evanescent field. Recent advances allow the fibers to be tapered to even smaller diameters, allowing more than 99% of the energy to be guided outside the fiber with effective field diameters of $\gtrsim 13 \lambda$ [1], bringing them up to typical Rydberg blockade radius sizes.

On this poster, we will present the current status of planning and building our new Nanofiber experiment such as the vacuum chamber and first tests of the nanofibers. We select Ytterbium due to its advantage of having the two-photon Rydberg excitation transitions close together with 399 nm and 395 nm, which simplifies the fiber design and is expected to have low thermal dephasing effects.

[1] R. Finkelstein *et. al.* Optica **8**, 208-215 (2021)

MO 12.5 Tue 14:00 Tent

Interfacing high overtone bulk acoustic wave resonators and Rydberg atoms in a 4K environment — ●SAMUEL GERMER, VALERIE MAUTH, CEDRIC WIND, JULIA GAMPER, WOLFGANG ALT, and SEBASTIAN HOFFERBERTH — Institute of Applied Physics, University of Bonn, Germany

Rydberg atoms possess electric dipole transitions over a large range of the electromagnetic spectrum and are therefore promising candidates for realizing hybrid quantum systems that bridge the microwave and optical regimes. We aim to realize such a hybrid system in which an electromechanical resonator mode can be cooled down to its quantum mechanical ground state via interactions with Rydberg atoms.

On this poster, we discuss the setup build of three parts, the magneto optical trap for Rubidium atoms, an ultra high vacuum chamber hosting the atom chip in a closed-cycle cryostat and a magnetic transport connecting both. The cryostat provides a 4K environment which is a prerequisite for cooling the high overtone bulk acoustic wave resonator (HBAR) close to its ground state and allows the use of superconducting components.

We present machine learning based optimization of the magneto optical trap and magnetic transport. Moreover, a first generation chip, consisting of a superconducting Z-wire trap and a microwave resonator, has been fabricated and characterization measurements are shown. For a second generation atom chip, featuring the HBAR, first simulations are presented which allow, among other things, to estimate the coupling strength between Rydberg atoms and the resonator.

MO 12.6 Tue 14:00 Tent

Cascaded Nonlinearities for Effectively Interacting Bose-Einstein Condensates of Photons — ●NIELS WOLF, ANDREAS REDMANN, CHRISTIAN KURTSCHIED, FRANK VEWINGER, JULIAN SCHMITT, and MARTIN WEITZ — Institut für Angewandte Physik, Bonn, Deutschland

Bose-Einstein condensation has been observed in ultracold atomic gases, polaritons, and, more recently, in low-dimensional photon gases. Since the photon-photon interaction is vanishingly small, thermalization of photons, e.g. as dye microcavity photon condensates in the latter systems, is achieved not through particle-particle collisions, but rather via contact with a reservoir, here the dye molecules [1]. Nevertheless, strong photon-photon interactions, such as effective Kerr interactions induced by cascaded second-order nonlinearities, could enable the realization of an interacting photon Bose-Einstein condensate. This could, e.g. open pathways to generating highly entangled photon states by purely thermodynamical methods [2]. We employ a triply resonant optical parametric oscillator setup with independent control over pump and subharmonic wavelength cavities. This config-

uration enables the generation of cascaded second-order nonlinearities, producing a phase shift potentially stronger than that of direct Kerr interaction. Suitable frequency filtering is crucial to tune the optical parametric oscillator to degeneracy, which is essential for fully characterizing the phase shift and determining the effective Kerr coefficient.

[1] J. Klaers et al., *Nature* 468, 545 (2010) [2] C. Kurtscheid et al., *Science* 366, 894 (2019)

MO 12.7 Tue 14:00 Tent

Evaluation of machine learning algorithms for applications in quantum gas experiments — ●OLIVER ANTON¹, ELISA DA ROS¹, PHILIPP-IMMANUEL SCHNEIDER^{3,4}, IVAN SEKULIC^{3,4}, SVEN BURGER^{3,4}, and MARKUS KRUTZIK^{1,2} — ¹Institut für Physik and IRIS, Humboldt-Universität zu Berlin — ²Ferdinand-Braun-Institut, Berlin — ³JCMwave GmbH, Berlin — ⁴Zuse Institute Berlin (ZIB), Berlin

The generation of clouds containing cold and ultra-cold atoms is a complex process that requires the optimization of noisy data in multi-dimensional parameter spaces. Optimization of such problems can present challenges both in and outside of the lab due to constraints in time, expertise, or access for lengthy manual optimization.

Machine learning offers a solution thanks to its ability to efficiently optimize high dimensional problems without the need for knowledge of the experiment itself. In this poster, we present the results of benchmarking various optimization algorithms and implementations. Their performance is tested in a cold atom experiment, subjected to inherent noise [1]. Current research aims towards the preparation of the cloud for quantum memory applications [2], by engineering the optical density using the tested algorithms.

[1] O. Anton et al., *Machine Learning: Science and Technology* 5 025022, 2024

[2] E. Da Ros et al., *Physical Review Research* 5 033003, 2023

MO 12.8 Tue 14:00 Tent

A Dipolar Quantum Gas Microscope in UV Optical Lattices — ●FIONA HELLSTERN, KEVIN NG, PAUL UERLINGS, MICHAEL WISCHERT, ALEXANDRA KÖPF, TANISHI VERMA, STEPHAN WELTE, RALF KLEMT, and TILMAN PFAU — 5. Physikalisches Institut and Center for Integrated Quantum Science and Technology IQST, Universität Stuttgart

We present progress on our dipolar quantum gas microscope, enabling in situ, single-atom, and single-site resolved detection of Dysprosium atoms in 180 nm spaced UV optical lattices. Using 360 nm light, we can create various lattice geometries to explore strongly correlated quantum phases. Due to the small lattice spacing, nearest-neighbor dipolar interactions can reach 200 Hz at 10 nK, granting us access to phases where long-range dipolar interactions play a dominant role.

UV spectroscopy has been performed to characterize key transitions, including isotope-specific features and a King plot analysis, essential for precise lattice control and future measurements. We present our results on the characterization of our high-NA (0.9) in-vacuum objective, highlighting its ability to achieve 180 nm spatial super-resolution through the implementation of shelving techniques. Finally, we outline our plans to leverage these tools for exploring novel quantum phases, dipolar many-body physics, and emergent phenomena in strongly interacting systems.

MO 12.9 Tue 14:00 Tent

Developing a quantum gas microscope with programmable lattices — SARAH WADDINGTON¹, ISABELLE SAFA¹, TOM SCHUBERT¹, ●RODRIGO ROSA-MEDINA¹, and JULIAN LÉONARD^{1,2} — ¹Atominstitut, TU Wien, Vienna, Austria — ²Institute of Science and Technology Austria (ISTA), Klosterneuburg, Austria

Experiments with ultracold atoms in optical lattices offer a versatile platform for engineering and probing strongly correlated quantum matter. While quantum gas microscopy has significantly advanced the field, enabling unprecedented single-site resolution, current experimental setups are often constrained by rigid lattice configurations and slow cycle times.

Here, we present our ongoing efforts to design and build a next-generation quantum gas microscope for fermionic and bosonic lithium atoms. Our approach relies on atom-by-atom assembly of small lattice systems employing auxiliary optical tweezers combined with all-optical cooling techniques to facilitate sub-second experimental cycles. By leveraging holographic projection techniques, we create tailored optical lattices with dynamically reconfigurable geometries. Our approach opens diverse research avenues, ranging from quantum simulation of

fractional quantum Hall states to frustrated phases with unconventional geometries.

MO 12.10 Tue 14:00 Tent

Cooling and trapping of Hg atoms with enhanced UV laser systems — ●RUDOLF HOMM and THOMAS WALTHER — Technische Universität Darmstadt, Institut für Angewandte Physik, Laser und Quantenoptik, Schlossgartenstraße 7, 64289 Darmstadt

The use of cold Hg atoms in a MOT offers a variety of experimental opportunities. The two stable fermionic isotopes are promising for a new time standard based on an optical lattice clock, using the ¹S₀ - ³P₀ transition at 265.6 nm. All stable isotopes can also form ultracold Hg dimers via photoassociation, combined with vibrational cooling.

Our setup includes two UV laser systems combined with a MOT for Hg atoms and a 2D-MOT for isotope preselection. Each laser system consists of a MOFA configuration, followed by two frequency-doubling stages.

The cooling laser provides a stable frequency and high power, generating over 1 W at 253.7 nm using Doppler-free saturation spectroscopy and an elliptical focus within the BBO crystal. The spectroscopy laser produces over 300 mW at 254.1 nm, mode hop free tunable over 16 GHz with a maximum scan rate of 3 Hz, using a feed-forward setup to stabilize the cavities.

We aim to achieve a high density of Hg atoms in the MOT to improve the signal for dimer spectroscopy. The latest results on trapping of Hg atoms with the improved UV laser systems will be presented.

MO 12.11 Tue 14:00 Tent

Correlation Functions for Interacting Fermi Gases in the BCS Regime — ●NIKOLAI KASCHEWSKI, SEJUNG YONG, and AXEL PELSTER — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Germany

Recent progress in developing quantum gas microscopes in the continuum [1-3] has opened new possibilities for detecting experimentally correlation functions in the realm of ultracold gases. Motivated by this, we present mean-field calculations of density-density correlation functions for interacting Fermi gases in the BCS regime.

Our results turn out to be strongly influenced not only by the temperature and the interaction strength for a harmonic confinement [4], but also by the effective range of the interaction in the homogeneous case [5]. As the latter has so far remained to be an elusive scattering parameter, its experimental detection via correlation function measurements is promising. This can shed new light on the prediction of two different superfluid phases for interacting Fermi gas [5].

[1] T. Jongh et al., arXiv:2411.08776 (2024).

[2] J. Xiang et al., arXiv:2411.08779 (2024).

[3] R. Yao, et al., arXiv:2411.08780 (2024).

[4] S. Yong et al., arXiv:2311.08853 (2023).

[5] N. Kaschewski, C. A. R. Sá de Melo, and A. Pelster, submitted for publication.

MO 12.12 Tue 14:00 Tent

Studying Dipolar Supersolids in Toroidal Geometries using DMDs — ●TANISHI VERMA¹, PAUL UERLINGS¹, FIONA HELLSTERN¹, KEVIN NG¹, ALEXANDRA KÖPF¹, MICHAEL WISCHERT¹, STEPHAN WELTE^{1,2}, RALF KLEMT¹, and TILMAN PFAU¹ — ¹5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Center for Integrated Quantum Science and Technology and CZS Center QPhoton, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Supersolids are characterised by a combination of the crystal structure of solids and the frictionless flow of superfluids, and can be realised experimentally through the self-organisation of long-range interacting trapped BECs into states of matter that resemble crystal like structures. In a recent work, dipolar supersolids in toroidal traps have been studied theoretically. Toroidal traps provide continuous rotational symmetry and periodic boundary conditions, which can be used to study the different amplitude and sound modes which emerge during the superfluid to supersolid phase transition, especially the Higgs amplitude mode, which has yet to be experimentally observed.

We plan to load the BEC produced in our new-generation Dysprosium machine in a toroidal trap made with a Digital Micromirror Device (DMD), and also implement a lightsheet using a 532nm laser for z-direction confinement. This poster presents our progress on the optical setup in order to create toroidal traps to study toroidal dipolar supersolids and their excitation modes.

MO 12.13 Tue 14:00 Tent

High-pressure xenon-noble gas mixtures as a thermalization mediator for VUV photons — ●THILO FALK VOM HÖVEL, ERIC BOLTERS DORF, FRANK VEWINGER, and MARTIN WEITZ — Institut für Angewandte Physik der Universität Bonn, Wegelerstr. 8, 53115 Bonn

In recent years, microcavity-based Bose-Einstein condensates of photons have become an established experimental platform. In these experiments, photons in the green-to-orange spectral range are confined to high-finesse microcavities filled with a liquid dye solution. Via repeated absorption and emission cycles, the photons adopt a thermal energy distribution, mediated by the thermalization of the dye molecules' rovibronic levels. Conveying these principles into the VUV spectral regime (100 - 200 nm) would allow for the construction of a coherent light source in a regime where the realization of a laser is difficult. For this endeavor, we intend to replace the dye molecules by a dense xenon-noble gas mixture, with xenon as the optically active constituent. For thermalization, we aim to exploit the transitions around a wavelength of 147 nm between the quasimolecular states associated with the (atomic) $5p^6$ and $5p^56s$ levels. We report on recent results on the spectroscopic investigation of such mixtures, with sample pressures of up to 100 bar. Centerpiece is a detailed study of absorption and emission spectra, with particular emphasis on the influence of the constituent partial pressures. The fulfillment of the thermodynamic Kennard-Stepanov relation is investigated, which constitutes an essential prerequisite for the suitability of a medium as a thermalization mediator for photons.

MO 12.14 Tue 14:00 Tent

Topological signatures in the dynamical response of periodically driven Su-Schrieffer-Heeger model — SOUMYA SASIDHARAN¹, ●SOURADEEP ROY CHOUDHURY², AHMET LEVENT SUBAŞI³, and NAVEEN SURENDRAN¹ — ¹Indian Institute of Space Science and Technology, Valiamala, Thiruvananthapuram-695547, India — ²Goethe-Universität, Institut für Theoretische Physik, 60438 Frankfurt am Main, Germany — ³Department of Physics, Faculty of Science and Letters, Istanbul Technical University, 34469 Maslak, Istanbul, Turkey

We study the dynamics of periodically driven Su-Schrieffer-Heeger model subjected to a range of driving conditions. In the large-amplitude, high-frequency regime, we establish a remarkable correspondence between the bulk dynamical response and the topology of the Floquet phase. At half-filling, we compute the dynamical order parameter Q , which is the time-averaged occupancy of an initially filled band. We show that Q is quantitatively related to a topological invariant. Furthermore, we obtain topologically protected edge states in the nontrivial phases.

MO 12.15 Tue 14:00 Tent

STIRAP for High Fidelity Spin-Flip in Ultracold ^6Li — ●ELLEN BRÄUTIGAM, CARL HEINTZE, SANDRA BRANDSTETTER, MACIEJ GALKA, and SELIM JOCHIM — Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany

We report on the implementation of Stimulated Raman Adiabatic Passage (STIRAP) in an ultra-cold few fermion ^6Li system. The atoms are transferred with high fidelity between the hyperfine states $|3\rangle$ and $|4\rangle$ in the ground state manifold. The transition is mediated via resonant coupling to an excited state in the D2 manifold while avoiding its population, ensuring negligible scattering and no atom loss. This method achieves robust and fast state transfer on the order of $1\mu\text{s}$, providing a reliable tool for precise quantum state control. Among other things, this allows us in combination with Feshbach resonance to perform a sudden interaction quench.

MO 12.16 Tue 14:00 Tent

Effects of dipolar cutoff shapes on numerical calculation of properties of dipolar condensates — ●DENIS MUJO¹ and ANTUN BALAZ^{1,2} — ¹Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia — ²Serbian Academy of Sciences and Arts

Here we study the impact of various shapes of dipolar cutoffs on the numerical calculation of ground state properties of dipolar Bose-Einstein condensates (BECs) and quantum droplets. In particular, we examine three distinct setups: the pure dipolar potential, where no cutoff is introduced; the analytically known spherical cutoff; and the cylindrical cutoff, that partially needs to be calculated numerically [1].

To understand how these different cutoff shapes affect the calculated values of physical properties of the ground state, we systematically vary key discretization parameters associated with each configuration. We demonstrate how the calculation precision of the cutoff translates into the precision of numerically obtained values of condensate and droplet properties.

[1] H.-Y. Lu et al., Phys. Rev. A **82**, 023622 (2010).

MO 12.17 Tue 14:00 Tent

Auto-ponderomotive beam manipulation for interaction-free measurements with electrons — ●FRANZ SCHMIDT-KALER¹, NILS BODE¹, FABIAN BÄMMES¹, MICHAEL SEIDLING¹, ROBERT ZIMMERMANN¹, JUSTUS WALTHER¹, LARS RADTKE¹, and PETER HOMMELHOFF^{1,2} — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — ²Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Cryo-electron microscopy achieves angstrom resolution for biological samples but requires reconstructing images from hundreds of thousands of identical molecules due to electron beam damage. *Interaction-free* measurements with electrons offer the potential for true single-particle analysis of radiation-sensitive samples. This method, already explored in the optical domain, requires developing electron-optical elements such as beam splitters, resonators, and guides. We present a resonator for 50 eV electrons, a guide for up to 9.5 keV electrons, and determine the first Matthieu stability regime for auto-ponderomotive devices. Our goal is to integrate these components into standard SEMs for broader applicability.

MO 12.18 Tue 14:00 Tent

Quantum gas microscopy of triangular-lattice Mott insulators — ●JAN DEPPE², LIYU LIU¹, JIRAYU MONGKOLKIATTICHA¹, DAVIS GARWOOD¹, JIN YANG¹, and PETER SCHAUSS² — ¹University of Virginia — ²Institute for Quantum Physics, University of Hamburg

This poster highlights our recent advances in the quantum simulation of electronic systems employing ultracold atoms in geometrically frustrated lattices. Frustrated quantum systems, known for hosting exotic phases like spin liquids, present a formidable challenge to condensed matter theory due to their extensive ground state degeneracy. Our focus centers on a triangular lattice, a paradigmatic example of geometric frustration where the degree of frustration is tunable. The triangular Hubbard model is a paradigm system for the study of kinetic frustration, which shows up in destructive interference between paths of holes, leading to antiferromagnetic polarons in hole-doped regime even at elevated high-temperatures. In our work, we showcase the realization of a Mott insulator of lithium-6 on a symmetric triangular lattice with a lattice spacing of 1003 nm. Spin removal techniques allow us to resolve individual spins and measure nearest neighbor spin-spin correlations across different interaction strengths. We find good agreement with numerical linked cluster expansion calculations and Quantum Monte Carlo simulations. Future endeavors involve the use of spin-resolved imaging through Stern-Gerlach splitting for full density and spin resolution. Additionally, exploration of bound states in strongly repulsive interacting systems is on the horizon.

MO 12.19 Tue 14:00 Tent

Polarization properties of Photon Bose Einstein Condensates — ●SVEN ENNS¹, JULIAN SCHULZ¹, KIRANKUMAR KARKIHALLI UMESH², FRANK VEWINGER², and GEORG VON FREYMAN^{1,3} — ¹Physics Department and Research Center OPTIMAS, RPTU Kaiserslautern Landau, Germany — ²Institut für Angewandte Physik, Universität Bonn, Germany — ³Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany

We experimentally investigate properties of harmonically trapped photon gases in a dye-filled microcavity. Specifically, we analyze the polarization of thermal and condensed light and their dependence on the polarization of the pump beam. Our experimental setup enables the creation of arbitrary polarization states on the Poincaré sphere for the pump beam. Additionally, the measurement basis can be switched from linear to circular polarization allowing for a proper evaluation of the photon gas's polarization by measuring fractions of two orthogonal polarization states simultaneously. In contrast to previous setups, the dye solution is pumped through the cavity mirrors and the pump beam coincides with the optical axis of the resonator so that no spontaneous symmetry breaking is expected. In agreement with previous theoretical work [1], there is a remarkable increase of the polarization

strength above the condensation threshold for a linear polarized pump. While the polarization of the condensate aligns with that of the pump beam, a circularly polarized condensate cannot be obtained. Below the condensation threshold, the photon gas stays unpolarized.

[1] R. I. Moodie, P. Kirton, and J. Keeling, *Phys. Rev. A* 96 (2017).

MO 12.20 Tue 14:00 Tent

Programmable Optical Lattices for Quantum Gas Microscopy — ●TOM SCHUBERT¹, ISABELLE SAFA¹, SARAH WADDINGTON¹, RODRIGO ROSA-MEDINA¹, and JULIAN LÉONARD^{1,2} — ¹Atominstitut, Technische Universität Wien, Austria — ²Institute of Science and Technology Austria (ISTA), Klosterneuburg, Austria

Creating tailored optical potentials on demand is crucial for quantum simulation experiments with ultracold atoms, supporting the exploration of diverse strongly correlated phenomena, such as magnetic frustration or topological order. In this poster, we present the design and projection of tuneable lattice potentials using holographic beam shaping methods, combined with precise corrections of optical aberrations. The corrections and projection of the potentials are achieved employing a Digital Micromirror Device (DMD) and a Spatial Light Modulator (SLM), which facilitate phase and amplitude modulation through the use of programmable diffraction gratings. Through the correction process, we enable phase correction of wavefront aberrations with resolutions on the order of $\lambda/100$. For shaping the corrected beam into the desired optical lattices, we implement different holographic projection methods, including basic Fourier Transform and the Gerchberg-Saxton algorithm, and analyze their performance. Further we implemented a versatile experiment control system (ARTIQ), employing FPGA hardware, facilitating real-time manual control of the SLM-DMD structure. As a result, we are able to implement a variety of optical potentials, ranging from lattices in box-shape potentials to linearly tilted superlattices.

MO 12.21 Tue 14:00 Tent

Stochastic phase noise in momentum-dependent Rabi oscillations — ●SAMUEL BÖHRINGER, FABIAN KIENLE, and RICHARD LOPP — Institut für Quantenphysik and Center for Integrated Quantum Science and Technology (IQST), Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

The laser-driven two-level system is the most fundamental model in quantum optics. It plays a central role in the description of beam splitters and mirrors in matter-wave interferometry and various other experiments with the ultimate goal to achieve high-precision measurements. A limiting factor to the precision of these measurements is laser phase noise. While there are numerous models for the description of laser phase noise in driven systems, they are lacking the inclusion of the center-of-mass (COM) degrees of freedom. However, the COM-motion is crucial for many applications. We provide a theoretical model for phase noise in Rabi oscillations including the COM degrees of freedom. In particular, we derive and solve a set of stochastic differential equations that describe the evolution of momentum-dependent observables during a laser pulse with phase noise.

MO 12.22 Tue 14:00 Tent

Extending the holographic superfluid model — ●MARTIN ZBORON¹, GREGOR BALS^{2,3}, THOMAS GASENZER^{1,2,3}, and CARLO EWERZ^{2,3} — ¹Kirchhoff-Institut für Physik, Uni Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg — ²Institut für Theoretische Physik, Uni Heidelberg, Philosophenweg 16, 69120 Heidelberg — ³ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

Gauge-gravity duality establishes a connection between strongly correlated quantum systems and higher-dimensional gravitational theories at weak coupling. Utilising an Abelian Higgs model in an asymptotically anti-de Sitter spacetime, one obtains the so-called holographic s-wave superfluid. A rich phenomenology is embodied in this model making dynamics of defects, such as quantised vortices, amenable to precise quantitative analysis. Aside from vortex dynamics in the dissipative superfluid, excitations like Kelvin waves on top of vortex lines can be studied as well as the instability of vortices with high winding numbers. Recent proposals presented possible extensions of the model in order to capture the transition to a holographic model of supersolidity, allowing access to dynamics of vortices as well as their pinning and unpinning within the supersolid state. This also opens a path to understanding the spin-down of pulsars in a supersolid framework.

MO 12.23 Tue 14:00 Tent

Optical dipole trapping of Rubidium in microgravity — ●MARIAN WOLTMANN, YANN SPERLING, JAN STIEHLER, MARIUS PRINZ, and SVEN HERRMANN — Center of Applied Space Technology and Microgravity (ZARM), University of Bremen, Germany

The sensitivity of atom interferometric sensors typically scales with the squared interrogation time. Therefore space-borne atom interferometry offers the potential of highly increased sensitivities that can be utilized for e.g. gravimetric measurements as well as for tests of fundamental physical principles.

Within the PRIMUS project we develop a compact all-optical matterwave source in a drop tower experiment. The all-optical approach utilizing a $\lambda = 1064$ nm crossed beam optical dipole trap enables the use of Feshbach resonances and offers the advantages of symmetric trapping potentials and magnetic substrate insensitive trapping. With our drop tower setup we demonstrated rapid Bose-Einstein condensation of ⁸⁷Rb with a minimum evaporation time of $t_{\text{evap}} = 1.3$ s to reach a critical phase space density on ground, while now focusing on the efficient preparation in microgravity. The PRIMUS-project is supported by the German Space Agency DLR with funds provided by the Federal Ministry for Economic Affairs and Climate Action under grant number DLR 50 WM 2042.

MO 12.24 Tue 14:00 Tent

Long-term stable laser injection locking for quasi-CW applications — ALEXANDRE DE MARTINO, FLORIAN KIESEL, ●KIRILL KARPOV, JONAS AUCH, and CHRISTIAN GROSS — Eberhard Karls Universität Tuebingen, Tuebingen, Germany

In our work we present a passive stabilization scheme for injection locking of high-power semiconductor laser diodes, that is generally applicable, technically easy to implement, and extremely cost-effective. It is based on the externally synchronized automatic acquisition of the optimal injection state. Central to our simple but powerful scheme is the management of thermalization effects during lock acquisition. By periodical relocking, spectrally pure amplified light is maintained in a quasi-CW manner over long timescales. We characterize the performance of our method for laser diodes amplifying 671nm light and demonstrate the general applicability by confirming the technique to work also for laser diodes at 401nm, 461nm, and 689nm. Our scheme enables the scaled operation of injection locks, even in cascaded setups, for the distributed amplification of single frequency laser light.

MO 12.25 Tue 14:00 Tent

Enhancing Rydberg Atom Cooling and Trapping with a Tunable Light Sheet — SHUANGHONG TANG, PHILIP OSTERHOLZ, SILPA BABURAJ-SHEELA, JULE BROSIG, ●LUKAS FISCHER, FABIO BENSCH, and CHRISTIAN GROSS — Eberhard Karls Universität Tübingen

The utilisation of Rydberg atoms trapped in optical tweezers provides a robust platform for the investigation of strongly interacting and correlated many-body systems. In order to facilitate the tunability of the trapping potential in the vertical direction, we implemented a thin light sheet. The tunability of the vertical confinement increases the trapping frequency, thereby facilitating Raman sideband cooling through the elevation of trap frequencies and the mitigation of gravitational forces, which allows for the implementation of shallower tweezers during the cooling process. A further challenge is the phenomenon of Talbot plane loading, which results in an undesired population of atoms in the planes adjacent to the tweezer array. To address this issue, the light sheet can be employed for loading, thereby ensuring that the atomic reservoir is confined to the primary tweezer plane.

MO 12.26 Tue 14:00 Tent

Pattern formation in dipolar quantum gases — ●ANDREEA-MARIA OROS¹, NIKLAS RASCH¹, WYATT KIRKBY^{1,2}, LAURIANE CHOMAZ², and THOMAS GASENZER^{1,3} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227 — ²Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 276 — ³Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16

Ultracold dipolar gases have garnered increasing interest over the past years. The anisotropic and long-range character of the dipolar interaction and the stabilizing nature of the quantum fluctuations give rise to supersolidity, superglasses, and exotic states of matter. Depending on the atom number, scattering length, and trapping geometry, different supersolid morphologies, such as triangular, honeycomb, and labyrinthine, have already been theoretically predicted to be the possible ground states of such a system. Our work expands on

these phases by considering the out-of-equilibrium dynamics of a harmonically trapped, three-dimensional dipolar condensate. Following a quench in the scattering length across a phase transition boundary, we investigate the dynamical formation of supersolids, and demonstrate quenches into the triangular, honeycomb, and labyrinth phases. We furthermore investigate systems which have artificially been brought out of equilibrium, such as systems with imprinted vortex ensembles, or where the initial state differs from one that could naturally occur, in order to better aid the search for non-thermal fixed points, as well as far-from-equilibrium and novel phenomena.

MO 12.27 Tue 14:00 Tent

Quantum gas microscopy of Rydberg-dressed extended Bose Hubbard models — ●DAVID GRÖTERS^{1,2,3}, PASCAL WECKESSER^{1,2}, KRITSANA SRAKAEW^{1,2}, DAVID WEI^{1,2}, DANIEL ADLER^{1,2}, SUCHITA AGRAWAL^{1,2}, IMMANUEL BLOCH^{1,2,3}, and JOHANNES ZEIHNER^{1,2,3} — ¹Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — ²Munich Center for Quantum Science and Technology (MC-QST), 80799 Munich, Germany — ³Fakultät für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany

The competition of different length scales in quantum many-body systems leads to various novel phenomena, including the emergence of correlated dynamics or non-local order. Off-resonant optical coupling to Rydberg states, known as Rydberg dressing, has been proposed as a versatile tool to engineer long-range interactions in lattice-based quantum simulators. So far however, this approach has been limited by collective losses, limiting Rydberg dressing to immobile spin systems.

On this poster, I present our recent findings on realizing an itinerant one-dimensional extended Bose Hubbard model using Rydberg-dressed ⁸⁷Rb atoms in optical lattices [1]. Here, we reduce the collective losses by two orders of magnitude using stroboscopic dressing. Harnessing our quantum gas microscope, we probe the correlated out-of-equilibrium dynamics of extended-range repulsively-bound pairs at low filling, and kinetically-constrained "hard rods" at half filling. Near equilibrium, we observe density ordering when adiabatically turning on the extended-range interactions.

[1] <https://arxiv.org/abs/2405.20128>

MO 12.28 Tue 14:00 Tent

Trapping and interfacing laser-cooled strontium atoms using an optical nanofibre — ●LUCA GÖCKE, HECTOR LETELLIER, PHILIPP SCHNEEWEISS, JÜRGEN VOLZ, and ARNO RAUSCHENBEUTEL — Department of Physics, Humboldt-Universität zu Berlin, Germany

We are in the process of building an experimental setup for trapping and optically interfacing laser-cooled strontium atoms using the evanescent field surrounding an optical nanofibre. The nanofibre is produced from a standard step-index optical fibre in a heat-pull process. It features a waist diameter of 200 nm where light is still efficiently guided while a significant part of the light propagates in the form of an evanescent field surrounding the nanofiber. Atoms are trapped in a one-dimensional (1D) optical lattice formed by two fiber-guided light-fields, red- and blue-detuned with respect to the strong transition at a wavelength of 461 nm. The aim is to realize a compensated trap, where the wavelengths of the trapping fields are magic for the 7.4 kHz wide intercombination line at 689 nm. This will allow us to implement advanced schemes for loading single atoms into the 1D optical lattice and to investigate the phenomenon of selective radiance [1], where the atoms themselves act as the waveguide. Here we will present our compact design for trapping strontium atoms from a laser ablated source with a "hot MOT" (operated at 461 nm wavelength), then transfer them to a "cold MOT" (operated at the intercombination line) and to the nanofibre trap.

[1]: A. Asenjo-Garcia et al. PRX 7, 031024 (2017)

MO 12.29 Tue 14:00 Tent

Fractal ground state of mesoscopic ion chains in periodic potentials — RAPHAEL MENU¹, JORGE YAGO MALO², ●JOSHUA WEISSENFELS¹, VLADAN VULETIC³, MARIA LUISA CHIOFALO², and GIOVANNA MORIGI¹ — ¹Universität des Saarlandes, Saarbrücken, Germany — ²Università di Pisa, Pisa, Italy — ³Massachusetts Institute of Technology, Cambridge, USA

Trapped ions in a periodic potential are a paradigm of a frustrated Wigner crystal. The dynamics is captured by a long-range Frenkel-Kontorova model. We show that the classical ground state can be mapped to the one of a long-range Ising spin chain in a magnetic field, whose strength is determined by the mismatch between chain's and substrate lattice's periodicity. The mapping is exact when the

substrate potential is a piecewise harmonic potential and holds for any two-body interaction decaying as $1/r^\alpha$ with the distance r . The ground state is a devil's staircase of regular, periodic structures as a function of the mismatch and of the interaction exponent α . While the staircase is well defined in the thermodynamic limit for $\alpha > 1$, for Coulomb interactions, $\alpha = 1$, we argue that it disappears and the sliding-to-pinned transition becomes a crossover, with a convergence to the thermodynamic limit scaling logarithmically with the chain's size. Due to this slow convergence, fractal properties can be observed even in chains of hundreds of ions at laser cooling temperatures.

MO 12.30 Tue 14:00 Tent

Lattice phase stabilization for a dipolar quantum gas microscope — ●ALEXANDRA KÖPF¹, FIONA HELLSTERN¹, KEVIN NG¹, PAUL UERLINGS¹, MICHAEL WISCHERT¹, TANISHI VERMA¹, STEPHAN WELTE², RALF KLEMT¹, and TILMAN PFAU¹ — ¹Physikalisches Institut and Center for Integrated Quantum Science and Technology IQST, Universität Stuttgart — ²Physikalisches Institut, Center for Integrated Quantum Science and Technology and CZS Center QPhoton, Universität Stuttgart

This poster presents the development of a dipolar quantum gas microscope using Dysprosium atoms, focusing on the critical role of optical lattice phase stabilization. Dysprosium atoms will be trapped and imaged in a 360 nm UV lattice, achieving nearest-neighbor dipolar interactions of approximately 200 Hz at 10 nK. Maintaining precise lattice stabilization is also essential to confine the atoms within the narrow depth of focus (approximately 260 nm) of the high-resolution in-vacuum objective (NA = 0.9). To achieve this, we use a 1064 nm infrared lattice for vertical confinement, complemented by an active phase stabilization scheme, stabilizing the lattice relative to the objective position. This setup employs FPGA-based boards to monitor and stabilize the lattice phase through a Michelson interferometer, ensuring robust atom confinement and alignment. This approach enables controlled, long-timescale investigations of dipolar quantum phenomena, offering new insights into strongly interacting quantum systems.

MO 12.31 Tue 14:00 Tent

A comparison of sub-Doppler cooling techniques using a nano-structured atom chip — ●KAI-CHRISTIAN BRUNS, JULIAN LEMBURG, JOSEPH MUCHOVO, VIVEK CHANDRA, SAM ONDRACEK, HENDRIK HEINE, and ERNST M. RASEL — Leibniz Universität Hannover, Institut für Quantenoptik

In the field of cold atomic physics, various sub-Doppler cooling techniques are being used. We investigate two different molasses cooling schemes using an atom chip with a nano-fabricated grating. These chips simplify and miniaturize quantum systems by enabling the trapping of atoms in a MOT with a single incident beam. Additionally, the use of grating atom chips also enhances the scalability and portability of such devices. These techniques holds promise for a wide array of applications, from fundamental research to practical implementations in earth observation.

In this poster, we compare sub-Doppler cooling of ⁸⁷Rb utilizing bright and gray molasses techniques. We manage to cool the atoms to 13 μ K and 5 μ K respectively. Additionally, we see an increase in phase-space density by a factor of three, when comparing gray molasses to bright molasses. To understand the benefits that this improvement could bring to experiments employing Bose-Einstein-condensates, we study the transfer into a magnetic trap.

MO 12.32 Tue 14:00 Tent

Double Bragg atom interferometry with Bose-Einstein condensates in microgravity — ●ANURAG BHADANE¹, DORTHE LEOPOLDT², PRIYANKA BARIK², GOVINDARAJAN PRAKASH³, JULIA PAHL⁴, SVEN HERRMANN³, ANDRE WENZLAWSKI¹, SVEN ABEND², MARKUS KRUTZIK^{4,5}, PATRICK WINDPASSINGER¹, ERNST RASEL², and THE QUANTUS TEAM^{1,2,3,4,6,7} — ¹JGU Mainz — ²LU Hannover — ³ZARM, U Bremen — ⁴HU Berlin — ⁵FBH Berlin — ⁶U Ulm — ⁷TU Darmstadt

The QUANTUS-2 device is a mobile, robust, high-flux atom interferometer utilizing ⁸⁷Rb, designed for microgravity environments such as those provided by the Bremen drop tower and Gravitower. The Gravitower enables higher repetition rates for experiments, establishing QUANTUS-2 as a testbed for future space-based missions.

Our experiment employs a magnetic lens via the quadrupole field of an atom chip, achieving extended coherence times and enabling interferometry durations exceeding one second with double Bragg diffraction under microgravity conditions. On this poster, we report recent

advancements in atom interferometry at extended timescales, along with the characterization of the system in the Gravitower.

This project is supported by the German Space Agency DLR with funds provided by the Federal Ministry for Economic Affairs and Climate Action under grant numbers DLR 50WM1952-1957 and DLR 50 WM 2450A-F

MO 12.33 Tue 14:00 Tent

Mean-field parton construction of Rydberg Quantum Spin Liquid from microscopic properties — ●BENNO BOCK, SIMON OHLER, and MICHAEL FLEISCHHAUER — RPTU, Kaiserslautern, Germany

Quantum Spin Liquids (QSL) represent an exotic phase of matter elusive to experiments. One hallmark property is the absence of magnetic spin order even at zero temperature. Despite numerous attempts, the unambiguous experimental confirmation of QSL states remains difficult. In this context, the possibility of realizing QSL physics on Rydberg atom-based quantum simulators has been a promising avenue for investigation [Semeghini et al., Science 374 (2021)].

Recently, the existence of a QSL state has been investigated numerically with Exact Diagonalization (ED) in a system of Rydberg atoms on a honeycomb lattice featuring density-dependent Peierls phases [Ohler et al., PRR 5 (2023)]. Later investigations using projective symmetry group arguments [Tarabunga et al., PRB 108 (2023)] confirmed the state to be a chiral spin liquid by comparing ground-states of ansatz Hamiltonians with ED results. In this work, we take a different approach, deriving explicitly the mean-field parton Hamiltonian starting from the microscopic Rydberg properties. We then determine the mean-field ground-state self-consistently, which yields a more accurate representation of the Rydberg ground-state. It shows large overlap with the ED simulation but is in principle not restricted to small system sizes.

MO 12.34 Tue 14:00 Tent

Aberration correction and trap creation in a dipolar quantum gas microscope — ●MICHAEL WISCHERT¹, KEVIN NG¹, FIONA HELLSTERN¹, PAUL UERLINGS¹, ALEXANDRA KÖPF¹, TANISHI VERMA¹, STEPHAN WELTE², RALF KLEMT¹, and TILMAN PFAU¹ — ¹Physikalisches Institut and Center for Integrated Quantum Science and Technology — ²Physikalisches Institut, Center for Integrated Quantum Science and Technology and CZS Center QPhoton, Universität Stuttgart

This poster focuses on calibrating and correcting optical aberrations as well as holographically projecting optical traps for a dipolar quantum gas microscope. To achieve large nearest-neighbor interactions (200 Hz at 10 nK), a 180 nm spaced near-UV lattice with dysprosium atoms will be used. This setup requires a high NA objective (NA 0.9) where minimizing imaging aberrations is critical for maintaining image fidelity. To mitigate these aberrations, we introduce a spatial light modulator (SLM) after the objective, enabling phase manipulation of the collected light and correction of the distorted wavefront. We test and compare different methods for calibrating and correcting aberrations using the SLM. Additionally, we explore the use of the SLM in creating tailored optical trap potentials by projecting and analyzing various trap geometries in a separate setup. Our work aims at exploring how SLMs can be utilized to improve imaging performance in quantum gas microscopes.

MO 12.35 Tue 14:00 Tent

Quantum turbulence in a dipolar Bose gas at the anomalous non-thermal fixed point — ●NIKLAS RASCH¹ and THOMAS GASENZER^{1,2} — ¹Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg — ²Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg

This work focuses on quantum turbulence in the vicinity of an anomalous non-thermal fixed point (NTFP) characterized by slow, subdiffusive coarsening of a length scale. The NTFP is approached in the temporal evolution of a quasi-2d dipolar Bose gas starting from variously sampled initial vortex configurations. Already in the early dynamics, we observe the build-up of an inverse energy cascade and recover Kolmogorov's $-5/3$ power law in the incompressible energy spectrum. Due to the irreversible conversion of incompressible (vortices) into compressible energy (sound) this is understood in the context of decaying turbulence. By studying higher moments of the velocity circulation, we aim to understand the role that intermittency plays in the approach to a non-thermal fixed point. Further, using the high tunability of the

anisotropic and long-range dipolar interaction we can probe its effects on the quantum turbulent behavior.

MO 12.36 Tue 14:00 Tent

Exploring extended Hubbard models in an optical superlattice — ●VALENTIN JONAS, NICK KLEMMER, JANEK FLEPER, AMENEH SHEIKHAN, CORINNA KOLLATH, MICHAEL KÖHL, and ANDREA BERGSCHNEIDER — Physikalisches Institut, Bonn, Germany

Ultracold atoms in optical lattices allow for simulating strongly correlated many-body systems in the Hubbard model. Its quantum phases arising from the interplay of tunneling and on-site interaction have been extensively studied over the last few years experimentally, while systems beyond the simple Hubbard model are much less explored.

Our experimental apparatus uses fermionic potassium atoms in a 3D optical lattice with an in-plane superlattice to realize chains of double wells. By asymmetrically shaking the double wells, we recently realized an effective Floquet system with additional pair tunneling while fully suppressing the dynamics of single particles. By controlling the drive frequency, we could tune the system and enhance pair tunneling up to the size of the superexchange [1].

Currently, we are investigating excited two-particle states in the superlattice such as repulsively bound atom pairs and can demonstrate their deterministic preparation in the double wells. These states are predicted to be connected to pair states featuring unconventional superconductivity.

[1] N. Klemmer et al., PRL (Accepted), 2024

MO 12.37 Tue 14:00 Tent

Reaction-Diffusion Dynamics of Quantum Gases — ●HANNAH LEHR, IGOR LESANOVSKY, and GABRIELE PERFETTO — Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

We consider the dynamics of quantum gases underlying coherent motion as well as dissipative reactions. For Fermions we discuss e.g., k-body losses $kA \rightarrow \emptyset$. In this case the universality lies within the long time decay of the particle density. For Bosons we consider also particle creating processes as branching $A \rightarrow A + A$. The competition between the latter and single body decay and coagulation $A + A \rightarrow A$ leads to an absorbing state phase transition in the stationary state. Our goal is to understand how quantum effects impact on the universality class of the transition.

We tackle these problems combining a variety of methods ranging from kinetic large-scale equations via the time-dependent generalized Gibbs ensemble method (TGGE), and Keldysh field-theory diagrammatic expansion. Specifically, for the Fermi gas under weak k-body losses we find long-time decay for the density of particles different from mean field. For the Bose gas, we observe a rich stationary phase diagram different from the classical counterpart of the model.

Our findings show that quantum effects impact on large-scale universal behaviour leading to novel universality classes compared to classical physics. These results are experimentally relevant since they directly connect to cold-atomic processes involving dissipative processes such as particle losses and creation.

MO 12.38 Tue 14:00 Tent

Single-Atom Addressing in Optical Lattices Using UV Raman Transitions — ●FRANCESCO TESTI^{1,4}, ANDREAS VON HAAREN^{1,2}, ROBIN GROTH^{1,2}, LUCA MUSCARELLA^{1,2}, JANET QUESJA^{1,2}, LIYANG QIU^{1,2}, IMMANUEL BLOCH^{1,2}, TIMON HILKER^{1,3}, TITUS FRANZ^{1,2,4}, and PHILIPP PREISS^{1,2} — ¹Max Planck Institute of Quantum Optics, Garching — ²Munich Center for Quantum Science and Technology — ³University of Strathclyde, Glasgow — ⁴Ludwig Maximilian University of Munich

FermiQP is a demonstrator for a lattice-based fermionic quantum processor utilizing ultracold fermions in optical lattices. Operating in analog mode, the system facilitates precision studies of the two-dimensional Fermi-Hubbard model. In its digital mode, it implements a universal gate set on the spin degree of freedom, enabling advanced state engineering and local basis transformations. Combined with a rapid preparation cycle for degenerate Fermi gases, FermiQP opens new pathways for fermionic quantum information processing, with applications in quantum chemistry and strongly correlated materials.

We present a single-atom addressing scheme for coherently manipulating the internal states of individual Lithium-6 atoms within an optical lattice. The scheme employs two-photon Raman transitions at a UV wavelength of 323 nm, optimizing atomic coherence while minimizing cross-talk to neighboring atoms. We provide a comprehensive

characterization of the 323 nm laser system and introduce an addressing system based on Acousto-Optic Deflectors capable of delivering up to six independently steerable beams in two dimensions.

MO 12.39 Tue 14:00 Tent

Challenges behind performing atom interferometry in extended free fall — ●PRIYANKA BARIK¹, DORTHE LEOPOLDT¹, ANURAG BHADANE², JULIA PAHL³, SVEN ABEND¹, SVEN HERRMANN⁴, ANDRÉ WENZLAWSKI², PATRICK WINDPASSINGER², MARKUS KRUTZIK^{3,7}, ERNST M. RASEL¹, and QUANTUS TEAM^{1,2,3,4,5,6,7} — ¹LU Hannover — ²JGU Mainz — ³HU Berlin — ⁴ZARM, U Bremen — ⁵U Ulm — ⁶TU Darmstadt — ⁷FBH Berlin

The QUANTUS-2 apparatus is a high-flux ⁸⁷Rb BEC machine, based on a magnetic chip-trap, which generates 1×10^5 atoms at a 1Hz rate. High-precision quantum sensing with atom interferometers requires long interrogation time of several seconds with ultra-low expansion rates of the BECs. Thus, we perform our experiment in the Drop Tower in Bremen with a novel matter-wave lens system for the collimation of the condensate. The QUANTUS-2 setup experiences noticeable tilts and rotations which alter the spatial rotation of the ⁸⁷Rb atomic cloud and its projection along the imaging axes and the interferometry pulses. These rotations lead to position offsets, which become more pronounced as the TOF is increased, and, hence, are expected to contribute to a loss of contrast of the interferometer. We report on the proposal to mitigate these problems using a retro-reflective mirror mounted on a tip/tilt platform which will pave the way for long interrogation times. This project is supported by the German Space Agency DLR with funds provided by the Federal Ministry for Economic Affairs and Climate Action under grant numbers DLR 50WM1952-1957 and DLR 50 WM 2450A-F.

MO 12.40 Tue 14:00 Tent

Design and characterization of a compact and transportable strontium MOT — ●DARIUS HOYER and SIMON STELLMER — Physikalisches Institut, Bonn, Deutschland

The broad linewidth of the $461 \text{ nm } (5s5s) ^1S_0 \rightarrow (5s5p) ^1P_1$ transition of strontium allows for efficient laser cooling and trapping in a magneto-optical trap (MOT). This results in a bright MOT that is visible to the naked eye. Thus the Sr MOT is an ideal toy model for making quantum optics more accessible to a wide audience. We present the design of a transportable Sr MOT based on permanent magnets for the Zeeman slower and the MOT.

MO 12.41 Tue 14:00 Tent

Rydberg interactions in ultracold Ytterbium — ●FLORIAN PAUSEWANG, TANGI LEGRAND, XIN WANG, LUDWIG MÜLLER, EDUARDO URUÑUELA, WOLFGANG ALT, and SEBASTIAN HOFFERBERTH — Institute of Applied Physics, University of Bonn, Germany

Mapping the strong interactions between Rydberg excitations in ultracold atomic ensembles onto photons opens the door to achieving high optical nonlinearities at the single-photon level. While previous demonstrations of this concept have relied exclusively on alkali atoms, two-valence-electron species like ytterbium offer unique advantages, such as narrow-linewidth laser cooling and, for Yb-174, potentially longer coherence times of polaritons compared to earlier Rubidium-based experiments. In this poster, we present our new ytterbium apparatus including Yb-specific challenges as light-induced atomic repulsion and two-photon ionization processes, and discuss our progress towards photon-photon interactions by Rydberg polaritons. We also report the spectroscopic characterization of ultra long-range Yb Rydberg molecules that arise as bound states in the low energy scattering of a highly excited Rydberg electron and a ground state atom. Our experimental setup featuring a dual-chamber compact design and a two-color MOT allows the creation of dipole trapped atomic ensembles at high density and low temperature, with $5 \cdot 10^6$ atoms and $T < 10 \mu\text{K}$ within 2s. Further evaporative cooling down to condensation is possible. Additionally, a field ionization system with ion detection via a Micro-Channel Plate enables high-precision spectroscopy.

MO 12.42 Tue 14:00 Tent

Toward Magnetically Insensitive ³⁹K BECs — ●WEI LIU, CONSTANTIN AVVACUMOV, ALEXANDER HERBST, ASHWIN RAJAGOPALAN, KNUT STOLZENBERG, DAIDA THOMAS, ERNST RASEL und DENNIS SCHLIPPERT — Leibniz Universität Hannover, Institut für Quantenoptik

The sensitivity of an atom interferometer(AI) is generally limited by

the standard quantum limit (SQL). Entangled interferometer schemes generated through atom-atom interactions in a trapped configuration can surpass the SQL, thereby enhancing the sensitivity of the AIs. However, trapped AIs are constrained by phase diffusion stemming from collisions at high atomic density. Feshbach resonances can suppress phase diffusion in trapped AI by tuning scattering length, enabling measurements with high-densities and large atomnumbers. ³⁹K BEC are ideal candidates for such interferometry schemes, as they feature broad resonances at low magnetic fields.

To create ³⁹K BEC in $m_F = 0$ suitable for AI at low field, the narrowness of resonance at 59.3G and spin-changing collision pose significant challenges for evaporative cooling. We present several schemes for generating a ³⁹K BEC in $m_F = 0$ through using microwave pulses and co-propagating Raman beam before and after evaporative cooling and discuss their limitations.

MO 12.43 Tue 14:00 Tent

Matter-wave interferometry with large metal clusters in a free-fall setup — ●ERIC VAN DEN BOSCH and KLAUS HORNBERGER — University of Duisburg-Essen, Germany

Matter-wave interferometry can be used to probe fundamental quantum properties on increasingly large scales. Using ionising gratings produced by UV lasers mitigates some of the limitations of material gratings, while also allowing for more versatile setups. We study an optical time-domain ionising matter-wave interferometer (OTIMA) setup [1] in a free-fall tower aimed at masses of up to 10^7 amu. We treat the influence of gravity and the Coriolis force in three dimensions and discuss possible experimental schemes to counteract the Coriolis effect.

[1] Nimmrichter, Haslinger, Hornberger, Arndt (2011). Concept of an ionizing time-domain matter-wave interferometer. *New Journal of Physics*, 13(7)

MO 12.44 Tue 14:00 Tent

Langevin dynamics of a Bose gas coupled to a small heat bath — ●CARSTEN HENKEL and SASHA ROEWER — Universität Potsdam, Institut für Physik und Astronomie

In an elongated, quasi-one-dimensional trap, a degenerate Bose gas is formed by atoms in the lowest quantum state of the “radial” confinement. Atoms in higher states can provide a heat bath which is, however, not much larger compared to the degenerate gas. We study with the help of Langevin dynamics (stochastic Gross-Pitaevskii equation) the evolution of the complex order parameter, taking into account the exchange of energy and particles with the heat bath. Curiously, as the heat bath gets smaller, its temperature drops, and the Bose gas is more degenerate. At the same time, temperature fluctuations are larger. Thermodynamically relevant quantities like the internal energy are extracted from the simulations. We also explore non-equilibrium situations with an externally imposed temperature difference.

MO 12.45 Tue 14:00 Tent

Symmetry-Preserving Condensation of Photons — ANDREAS REDMANN, ●RICCARDO PANICO, FRANK VEWINGER, JULIAN SCHMITT, and MARTIN WEITZ — Institut für Angewandte Physik, Universität Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

We investigate the statistical behavior of a Bose-Einstein condensate of photons in a dye-filled optical microcavity. This system enables the observation of grand-canonical statistical conditions through the coupling of photons to a reservoir of dye molecules, supporting the coexistence of macroscopic occupation and unusually large fluctuations of the particles number. Building on prior demonstrations of grand-canonical statistics [1,2], we push the boundaries of our system to explore conditions for which the first- and second-order coherence times become comparable. In this regime, the condensate exhibits a discontinuous phase, driven by the relatively high probability of having zero particles in the condensate, with spontaneous emission of photons from the reservoir setting the phase of the condensate each time. Despite this, photons are expected to exhibit macroscopic occupation on average, while at the same time having characteristics of incoherent light sources. From a thermodynamic perspective, this would translate to the formation of a condensate without spontaneous symmetry breaking.

[1] Julian Schmitt, et al., *Laser Spectroscopy*, pp. 85-96 (2016)

[2] Julian Schmitt, et al., *Phys. Rev. Lett.* **116**

MO 12.46 Tue 14:00 Tent

Assessing interactions of Rb vapor with mirror coatings for compact cold-atom sources — ●CONSTANTIN AVVACUMOV,

ALEXANDER HERBST, WEI LIU, ASHWIN RAJAGOPALAN, KNUT STOLZENBERG, DAIDA THOMAS, ERNST RASEL, and DENNIS SCHLIPPERT — Leibniz Universität Hannover, Institut für Quantenoptik

Atom interferometers are effective tools for fundamental research and geodesy applications, e.g. for gravimetry. Fundamentally, quantum projection noise motivates the development of high-flux cold atom sources. A typical first cooling stage of atom interferometers is a two-dimensional magneto-optical trap (2D-MOT). In recent years, attempts to improve on 2D-MOTs' SWaP (size, weight, and power) budget raised questions regarding the compatibility of high-quality optical coatings exposed to alkali vapor, e.g., rubidium or potassium.

In this poster, we present systematic analysis of the interaction of Rb vapor with highly reflective coating materials (gold, silver, aluminium, dielectric coatings) and compare samples with and without protective coating. In our mirror testing setup, we observe mirror reflectivity degradation as a function of time and Rb partial pressure in a long-term perspective. Six mirror samples are exposed to alkali vapor at partial pressures up to and about saturation level (about $5 \cdot 10^{-7}$ mbar at room temperature). The results show significant reduction in mirror lifespan at Rb pressures above saturation level, which varies, however, for different samples. Analysis of the reactivity of alkali vapor with various materials at different pressures has an application in design of future compact quantum optical experiments.

MO 12.47 Tue 14:00 Tent

Local Chern number for noninteracting fermions in the Haldane model with external confinement — DANIEL SAMOYLOV and WALTER HOFSTETTER — Goethe Universität, Institut für Theoretische Physik, 60438 Frankfurt, Germany

We numerically study the formation of topological domains in the Haldane model on a honeycomb lattice in the presence of an external trapping potential. To map out topological domains in real space we calculate the local Chern number of the system as a function of position. The local Chern number was introduced by Bianco and Resta [1] as a topological marker of the Chern number. In order to test our implementation, we calculate the local Chern number of the Haldane model without external potential and confirm the results in [1]. By adding an external potential to the system, we find different topological domains which are indicated by a spatial variation of the local Chern number across the honeycomb lattice. We investigate the formation of topologically non-trivial domains, both as a function of the Fermi energy and for different shapes of the trapping potential. Related results were obtained for the Hofstadter model in [2].

[1] R. Bianco and R. Resta, Phys. Rev. B 84, 24 (2011)

[2] U. Gebert, B. Irsigler, and W. Hofstetter, Phys. Rev. A 101, 6 (2020)

MO 12.48 Tue 14:00 Tent

Laser-induced lattice potentials for optical quantum gases inside microcavities — PURBITA KOLE¹, NIKOLAS LONGEN¹, DANIEL EHRMANNTRAUT¹, PETER SCHNORRENBERG¹, KEVIN PETERS¹, and JULIAN SCHMITT^{1,2} — ¹Universität Bonn, IAP, Wegelerstr. 8, 53115 Bonn — ²Universität Heidelberg, KIP, Im Neuenheimer Feld 227, 69120 Heidelberg

Lattice potentials provide a fundamental ingredient for the description and study of the behaviour of particles in crystal-like structures, most notably in condensed matter systems. The realisation of photon Bose-Einstein condensates in arrays of coupled dye-filled microcavities opens a new platform for such physics owing to the high degree of tunability of the potentials in 1D and 2D. Here, we present laser-induced reversible and irreversible mirror structuring techniques for the generation of periodic lattice potentials for photon Bose-Einstein condensates with variable site-resolved control of the potential energy. As the dispersion relation for the two-dimensional photon gas inside an optical dye-filled microcavity depends on the cavity length, static potentials are introduced by modulating the mirror surface with a laser writing method. Harnessing the thermo-optic effect in the dye solution, we then modify the optical path length in a reversible way by projecting structured light onto an absorbing Si-layer in the backside of one of the cavity mirrors. The two-fold tuning of lattice potentials opens the possibility to study a variety of novel Hermitian and non-Hermitian effects with quantum gases of light.

MO 12.49 Tue 14:00 Tent

Fast 24-bit analog-to-digital converter for high-precision experiment control — JONAS DROTLEFF, PHILIPP LUNT, JOHANNES REITER, PAUL HILL, MACIEJ GAŁKA, and SELIM JOCHIM —

Physikalisches Institut der Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany

Cold atom experiments rely on precision measurements and stable experimental parameters to prepare and control quantum states with high fidelity. High-dynamic range analog-to-digital converters (ADCs) minimize the information loss caused by the digitalization and play a major role in modern experiment control systems. We present a novel measurement device that provides a large dynamic range (19 noise-free bits) at sampling rates of up to 2 million samples per second. At lower sampling rates, the converter yields up to 24 noise-free bits, allowing for enhanced flexibility in the type and bandwidth of input signals. With its small and portable design, the device allows for digitalization close to the signal's origin, thereby eliminating long signal paths and subsequent noise pickup. This ADC is the first step towards more precise control of experimental parameters, with potential applications in the range from ultra-precise stabilization of optical trap depths to magnetic offset field control at unprecedented levels.

MO 12.50 Tue 14:00 Tent

Towards trapping of single atoms in a micro-fabricated optical tweezer — MARIAN ROCKENHÄUSER¹, LUKAS BLESSING², and TIM LANGEN¹ — ¹TU Wien, Atominstitut, Cold Molecules and Quantum Technologies — ²Universität Stuttgart, 5. Physikalisches Institut

The trapping of single ultracold atoms is a crucial technique for applications in quantum computation, communication, and sensing. However, one of the main disadvantages of most experiments is their considerable large size and complexity. Here we present our progress towards the miniaturization of a classic single atom experiment. This is achieved by the use of a sophisticated compact laser system and the integration of a 3D-printed optical tweezer with a rubidium magneto-optical trap. The tweezer is created using micrometer-scale lenses fabricated directly onto the tip of a standard optical fiber. These unique properties enable the efficient trapping of single atoms and the collection of their fluorescence using the same fiber. Its unique properties will make it possible to both trap single atoms and the subsequent collection of their fluorescence with high efficacy. Based on this, a single-photon source can be realized which will have extensive applications in the field of quantum information processing.

MO 12.51 Tue 14:00 Tent

Quantum simulation and computation using fermions in an optical superlattice — MARNIX BARENDREGT¹, THOMAS CHALOPIN^{1,2}, PETAR BOJOVIĆ¹, SI WANG¹, JOHANNES OBERMEYER¹, DOMINIK BOURGUND¹, TITUS FRANZ¹, IMMANUEL BLOCH¹, and TIMON HILKER^{1,3} — ¹Max Planck Institute of Quantum Optics, Garching, Germany — ²Université Paris-Saclay, Institut d'Optique Graduate School, CNRS, Laboratoire Charles Fabry, Palaiseau 91127, France — ³Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK

Strongly-correlated materials show rich phase diagrams at low temperatures and finite dopings. The Fermi-Hubbard model and its variations are believed to describe many of these phases, including cuprate high-Tc superconductivity and the pseudogap phase. We have implemented a single-site and spin resolved quantum gas microscope with an optical superlattice. Control over the doping and temperature has allowed us to explore large regions of the Fermi-Hubbard phase diagram and find indications of the pseudogap phase by measuring spin and dopant-spin correlations up to fifth order. Additionally, atoms in the superlattice can be isolated into an array of double wells, which we dynamically control to implement two-qubit collisional gates with excellent fidelity. This paves the way for fermionic quantum computation.

MO 12.52 Tue 14:00 Tent

Experimental Study of the Solidity and Smecticity of a Driven Superfluid — NIKOLAS LIEBSTER, MARIUS SPARN, ELINOR KATH, JELTE DUCHENE, HELMUT STROBEL, and MARKUS OBERTHALER — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Bosonic quantum gases have been shown to result in spontaneously arising, self-stabilized periodic density modulations when the two-particle interaction strength is driven in time. Here we experimentally demonstrate that such states share key properties to a seemingly different physical system, namely supersolids, not only in their superfluidity and periodic density structure but also in their excitations. This correspondence is made possible through the effective theory of hydrodynamics of supersolids, which is constructed using assumptions of

spontaneously broken symmetries and conserved quantities. We experimentally investigate both stripe patterns as well as two-dimensional crystals, using novel techniques to instigate sound modes in each configuration.

MO 12.53 Tue 14:00 Tent

Realization and characterization of a tunable 2D optical accordion for ultracold atoms — ●KRISHNAN SUNDARARAJAN, ALEXANDER GUTHMANN, FELIX LANG, LOUISA MARIE KIENESBERGER, and ARTUR WIDERA — Physics Department and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany

Optical lattices, formed by the interference of coherent laser beams, are powerful tools for manipulating quantum gases. A versatile implementation, the optical "accordion," enables tuneable lattice spacing by adjusting the angle between beams. We aim to develop such a setup using a beam splitter made of custom Dove prisms bonded with UV-curing epoxy, combined with a large aspherical lens. The prism pair splits a single beam into two parallel rays, whose separation depends on the incoming beam properties. Focusing these rays creates an interference pattern forming the lattice potential. We will present the design, assembly, and ex-situ characterization of this optical accordion and its extension to a 2D configuration for accessing lower-dimensional systems with ultracold lithium-6 atoms.

MO 12.54 Tue 14:00 Tent

Two-dimensional grating magneto-optical trap — ●JOSEPH MUCHOVO, JULIAN LEMBURG, SAM ONDRACEK, KAI-CHRISTIAN BRUNS, VIVEK CHANDRA, HENDRIK HEINE, and ERNST M. RASEL — Leibniz Universität Hannover, Institut für Quantenoptik

Ultracold atoms provide exciting opportunities for advancing matter-wave interferometry and enabling more precise tests of fundamental physics in a variety of experimental and applied settings. To achieve larger atom numbers and higher repetition rates, two-dimensional (2D) magneto-optical traps (MOTs) can be employed as separate source chambers. These offer distinct advantages in the pre-cooling and faster, more efficient loading of atoms into three-dimensional grating MOTs, a key step for many precision measurements. To realise field applications of quantum sensors utilising cold atoms, there is need for simpler, more efficient and more compact sources.

In this poster, we will present the design and implementation of a 2D grating MOT requiring only a single input cooling beam in combination with pusher-retarder beams, thereby simplifying the setup. This innovative approach will result in a robust, highly compact, and efficient source of ultracold atoms that can be used in field and space applications.

MO 12.55 Tue 14:00 Tent

Developing a hybrid tweezer array of Rydberg atoms and polar molecules — ●KAI VOGES, DANIEL HOARE, JOE VAGGE, QINSHU LYU, JONAS RODEWALD, BEN SAUER, and MICHAEL TARBUTT — Centre for Cold Matter, Imperial College London, UK

Hybrid tweezer arrays of atoms and molecules are an innovative tool for new applications in quantum science and technology. The combination of Rydberg atoms with their large electric dipole moment and polar molecules with their rich level structure and long state coherence times makes this approach a promising platform for quantum simulation [1] and computing [2,3].

In this poster, we show our recent results on the realization of such a hybrid tweezer array based on ultracold Rb atoms and directly laser-coolable CaF molecules. We discuss the advantages and challenges of using two different ultracold particle types and present our preparation strategies for the atoms and molecules. In addition, we show our results in single atom trapping, imaging and tweezer trap characterisation and present our progress for highly efficient tweezer loading. Our approach will make it possible to construct arbitrary patterns of atoms and molecules. Through the dynamic rearrangement of tweezers and the long-range interactions mediated by Rydberg atoms, this hybrid platform will be a compelling candidate for scalable quantum computing.

- [1] J. Dobrzyniecki et al., PRA 108, 052618 (2023)
- [2] C. Zhang et al., PRX Quantum 3, 030340 (2022)
- [3] K. Wang et al., PRX Quantum 3, 030339 (2022)

MO 12.56 Tue 14:00 Tent

Observation of an integer quantum Hall state of six fermions — ●JOHANNES REITER, PAUL HILL, PHILIPP LUNT, JONAS DROTL-
EFF, MACIEJ GALKA, and SELIM JOCHIM — Physikalisches Institut,

Universität Heidelberg, Deutschland

Integer and fractional quantum Hall states underpin the understanding of topological phases of matter featuring exotic macroscopic properties such as the quantization of the transverse resistivity and emergence of robust edge currents.

Expanding upon our deterministic preparation of a spinful two-particle Laughlin state [arXiv:2402.14814], we present the recent observation of an integer quantum Hall state of six rapidly rotating fermions confined in a tight optical tweezer. Momentum-space imaging of the many body density reveals the hallmark uniform flattening of the particle density distribution and provides access to the microscopic correlations. This measurement demonstrates the scalability of our atom-by-atom assembly technique of quantum hall states and opens new avenues for probing the microscopic dynamics of topological phase transitions.

MO 12.57 Tue 14:00 Tent

Exploring the superfluid phase diagram for imbalanced Fermi gases in 2D — ●RENÉ HENKE, CESAR R. CABRERA, MORITZ VON USSLAR, ARTAK MKRTCHYAN, and HENNING MORITZ — Institut für Quantenphysik, Universität Hamburg

In Fermionic superfluids, condensation occurs through the pairing of fermions with opposite momenta and spin. This process is disturbed by introducing a spin imbalance, which leads to a mismatch between the respective Fermi surfaces. The result is a complex phase diagram including different phases, such as phase separation between a balanced superfluid and free fermions, as well as more exotic phases like the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, where the pairs carry non-zero momentum. As of now, the phase diagram of imbalanced Fermi gases in two dimensions remains largely unexplored.

In this poster, we present our results on spin-imbalanced homogeneous Fermi gases in two dimensions. Using lattice modulation spectroscopy, we excite a collective mode associated to the superfluid order parameter of the system. Our results show how this collective mode vanishes at a critical polarization and interaction strength, providing a step towards understanding exotic pairing in low dimensions.

MO 12.58 Tue 14:00 Tent

Towards a Potassium-39 quantum gas microscope — SCOTT HUBELE, ●YIXIAO WANG, MARTIN SCHLEDERER, ALEXANDRA MOZDZEN, GUILLAUME SALOMON, and HENNING MORITZ — Institute for Quantum Physics, University of Hamburg, Germany

The rapid development of quantum simulation has enabled us to study many-body physics with cold atom experiments in a controlled way, avoiding the computational complexity of solving the problems with classical computers. The introduction of quantum gas microscopes further allows to study the system with single-site resolution in real space.

In our experiment, we prepare ultracold Potassium-39 in a 1064nm optical lattice in a bowtie configuration, which can be well described by the Bose-Hubbard model, and confine the atoms in quasi-2D geometry with a pancake-shaped trap and a vertical repulsive lattice. To achieve single-site resolution, we employ Raman sideband imaging at near-zero magnetic field to cool the atoms while simultaneously collecting fluorescence photons with a high-NA objective.

Here, we present the progress towards building a Potassium-39 quantum gas microscope and introduce the experimental techniques for preparing ultracold atoms in the optical lattices and imaging them with high resolution using Raman sideband imaging.

MO 12.59 Tue 14:00 Tent

An experimental study of the heating of laser-cooled atoms in a nanofiber-based two-color trap — ●ANTOINE GLICENSTEIN, RICCARDO PENNETTA, DANIEL LECHNER, JÜRGEN VOLZ, PHILIPP SCHNEEWEISS, and ARNO RAUSCHENBEUTEL — Department of Physics, Humboldt-Universität zu Berlin, 10099 Berlin, Germany

The lifetime of atoms in nanofiber-based optical traps is significantly smaller than in comparable free-space traps. This experimental observation has been made for different types of trapped atoms such as Cesium or Rubidium, and the mechanical motion of the nanofiber has been proposed to be the major factor behind the excess heating [1]. By analyzing the polarization fluctuations of light transmitted through the nanofiber, we observe the nanofiber's fundamental torsional mode [2], which exhibits a Q-factor of up to 10^7 and a resonance frequency close to the trapping frequencies. In order to study its potential influence on the atoms' lifetime, a piezo actuator is integrated into the

nanofiber holder. While we successfully implemented feedback cooling to suppress the torsional motion and actively drove the torsional mode, neither approach resulted in a significant modification of the lifetime, indicating that the torsional mode is irrelevant for the heating rate of trapped atoms. Our research now shifts to investigating flexural modes, which are theoretically predicted to contribute most strongly to the heating [1] but are experimentally more challenging to address.

[1] Hümmer et al., PRX 9, 041034 (2019) [2] Tebbenjohanns et al., PRA 108, L031101 (2023)

MO 12.60 Tue 14:00 Tent

Possible configurations of the Heidelberg Quantum Architecture — •DANIEL DUX, TOBIAS HAMMEL, MAXIMILIAN KAISER, MATTHIAS WEIDEMÜLLER, and SELIM JOCHIM — Physikalisches Institut, Heidelberg, Germany

We present the current status of our new modular Lithium-6 platform. Besides a high degree of adaptability, this platform aims for a very fast cycle rate. We show first results from some of the already implemented modules, such as dipole traps, optical tweezers, an optical accordion to provide a 2D confinement, RF coils that enable fast spin flips, a free space imaging setup that allows simultaneous spin selective readout and a self optimization routine to set experiment parameters. Given these modules, we will discuss possible configurations that will be achievable within the Heidelberg Quantum Architecture and find applications in quantum technologies.

MO 12.61 Tue 14:00 Tent

Deterministic Generation of Localized Spin Excitations in a Spin-1 BEC — YANNICK DELLER, •ALEXANDER SCHMUTZ, RAPHAEL SCHÄFER, ALEXANDER FLAMM, HELMUT STROBEL, and MARKUS K. OBERTHALER — Kirchhoff-Institut für Physik, Universität Heidelberg, Deutschland

We present the experimental techniques to reliably generate localized spin excitations in a quasi one-dimensional ferromagnetic spin-1 BEC. We utilize a steerable laser at the tuneout-wavelength for ^{87}Rb in order to locally induce an effective magnetic offset field which can be controlled on the μm scale. Localized transitions between hyperfine states are implemented by amplitude modulation of the laser beam at the transition frequency [1].

To characterize the resulting spin excitations, we track their time evolution in all relevant observables by employing a generalized POVM readout scheme [2].

We investigate their properties such as lifetime and propagation speed in different parameter regimes and compare with numerical simulations and analytical models to investigate for a topological classification of the excitations.

1 Lannig et. al., PRL 125, 170401 (2020)

2 Kunkel et. al., PRL 123, 063603 (2019)

MO 12.62 Tue 14:00 Tent

Heidelberg Quantum Architecture - Fast and modular quantum simulation — •FINN LUBENAU, MAXIMILIAN KAISER, DANIEL DUX, TOBIAS HAMMEL, MATTHIAS WEIDEMÜLLER, and SELIM JOCHIM — Physikalisches Institut der Universität Heidelberg, Heidelberg, Germany

We are presenting our Heidelberg Quantum Architecture, a quantum gas platform that combines individual modules to implement a large variety of functionalities, that can be quickly updated and exchanged.

Currently, the core modules consist of a cold atom source that allows for very fast cycle time, dipole traps and optical tweezers, high fidelity single atom and spin resolved imaging, confinement to a 2D plane using an optical accordion. Here we will present progress on implementing a spatial light modulator (SLM) module to create tunable light fields in a precise and reproducible way, including the ability to correct for optical aberrations.

MO 12.63 Tue 14:00 Tent

ORKA - Towards a Cavity Enhanced All Optical Rb87 BEC Source for Atom Interferometry in Microgravity — •JAN ERIC STIEHLER, MARIUS PRINZ, MARIAN WOLTMANN, and SVEN HER-

RMANN — Center of Applied Space Technology and Microgravity (ZARM), University of Bremen, Germany

Evaporative cooling in optical traps is a common method to prepare ultra-cold atoms and generate Bose-Einstein-condensates (BEC). This usually comes at the price of an increased power budget for the trapping lasers. For setups that require energy efficiency, e.g. in space, magnetic chip traps are thus often preferred. However, these also come with their own limitations and lack some of the benefits of all-optical trapping and cooling. As an alternative, we are investigating the use of a resonantly enhanced 1064nm optical dipole trap for Rb87 to mitigate the power needs for all optical evaporative cooling. We are working on employing a bow-tie cavity for evaporative cooling down to a BEC to then be used as a matterwave source for interferometry in free-fall experiments at the Gravitower Bremen facility. Here we present our design and current progress of the experiment as well as first tests of the resonator. The ORKA project is supported by the German Space Agency DLR with funds provided by the Federal Ministry for Economic Affairs and Climate Action under grant number DLR 50 WM 2267.

MO 12.64 Tue 14:00 Tent

Ground Support for the BECCAL Laser System for Cold Atom Experiments onboard the ISS — •HAMISH BECK¹, HRUDYA THAIVALAPPIL SUNILKUMAR¹, MARC KITZMANN¹, MATTHIAS SCHOCH¹, CHRISTOPH WEISE¹, BASTIAN LEYKAUF¹, EVGENY KOVALCHUK¹, JAKOB POHL¹, ACHIM PETERS¹, and THE BECCAL COLLABORATION^{1,2,3,4,5,6,7,8,9,10} — ¹HUB, Berlin — ²FBH, Berlin — ³JGU, Mainz — ⁴LUH, Hanover — ⁵DLR-SI, Hanover — ⁶DLR-QT, Ulm — ⁷UULM, Ulm — ⁸ZARM, Bremen — ⁹DLR, Bremen — ¹⁰DLR-SC, Braunschweig

The Bose-Einstein Condensate and Cold Atom Laboratory (BECCAL) is designed for operation onboard the International Space Station (ISS). This multi-user facility will enable experiments with K and Rb ultra-cold atoms and BECs in microgravity. Fundamental physics will be explored at longer time- and lower energy-scales compared to those achieved on earth.

The BECCAL laser system is comprised of micro-integrated diode lasers, miniaturized free-space optics on Zerodur boards, and a system of fibres to bring light to the physics package. The design is subject to strict size, weight, and power (SWaP) constraints, and the operation of the system is supported by extensive ground-based systems.

The ground-based systems built for validation and testing will be presented alongside the design of the flight model.

This work is supported by the DLR with funds provided by the BMWK under grant number 50WP2102.

MO 12.65 Tue 14:00 Tent

Kármán vortex streets in a dissipative superfluid — •GEORG TRAUTMANN¹, GREGOR BALS^{2,3}, THOMAS GASENZER^{1,2,3}, CARLO EWERZ^{2,3}, and DAVIDE PROMENT^{3,4,5} — ¹Kirchhoff-Institut für Physik, Uni Heidelberg — ²Institut für Theoretische Physik, Uni Heidelberg — ³ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung — ⁴School of Engineering, Mathematics and Physics, University of East Anglia, Norwich Research Park — ⁵Centre for Photonics and Quantum Science, University of East Anglia

Moving an obstacle potential in a two-dimensional Bose-Einstein condensate can lead, depending on the potential's size and velocity, to different phases of vortex shedding. Of particular interest is the formation of a long-lived alternating series of vortex pairs with the same winding number, similar to the Bérnard-von Kármán vortex street known from classical fluid dynamics. Furthermore, simulating the vortex dynamics in a dissipative framework allows one to compare observations to a holographic superfluid where the strongly correlated quantum system is modeled through a higher-dimensional, weakly coupled gravitational theory. Recent literature has already shown successfully that the trajectories of simple vortex configurations simulated by dissipative Gross-Pitaevskii equations can be matched to the holographic analog. On the experimental side, the strongly dissipative quantum fluid can also describe liquid helium close to the lambda-transition qualitatively. Additionally, strong dissipation gives rise to further phases of vortex shedding that are not present in the non-dissipative condensate.

MO 13: Ultrafast Dynamics II

Time: Wednesday 11:00–13:00

Location: HS XVI

MO 13.1 Wed 11:00 HS XVI

Photo-induced structural dynamics of thymine with ultrafast electron diffraction — ●XIAOJUN WANG¹, JACKSON LEDERER², DENNIS MAYER¹, FABIANO LEVER¹, PEDRO NUNES², YUSONG LIU³, SURJENDU BHATTACHARYYA³, NIKHIL PACHISIA², XINXIN CHENG³, TIANZHE XU³, STEPHEN WEATHERSBY³, RANDY LEMONS³, PATRICK KRAMER³, PHILIPP LENZEN³, MING-FU LIN³, KIRK LARSEN³, FUHAO JI³, ROBERT ENGLAND³, CHRISTINA HAMPTON³, BRIAN KAUFMAN³, ALICE GREEN³, ALEXANDER REID³, TODD MARTINEZ^{3,4}, THOMAS WOLF³, MARTIN CENTURION², and MARKUS GUEHR^{1,5} — ¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, USA — ³SLAC National Accelerator Laboratory, Menlo Park, USA — ⁴Department of Chemistry, Stanford University, Stanford, USA — ⁵Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany

The photoprotection mechanism of thymine involves complex relaxation dynamics, where energy from photoexcitation is converted into vibrational energy through radiationless transitions. Previous studies have indicated that isolated thymine molecules undergo $^1\pi\pi^* \rightarrow ^1n\pi^*$ internal conversion within 100 femtoseconds (fs), followed by the intersystem crossing from $^1n\pi^*$ to the triplet state within 10 picoseconds (ps). However, the nuclear dynamics accompanying the transitions have not been experimentally resolved. Here we present a direct observation of the ultrafast nuclear motions using ultrafast electron diffraction, on the fs timescale and sub-Ångstrom resolution.

MO 13.2 Wed 11:15 HS XVI

Ultrafast electron diffraction imaging of wavelength-dependent trans-to-cis isomerization in azobenzene — SURJENDU BHATTACHARYYA¹, MING-FU LIN¹, THOMAS J. A. WOLF¹, ALICE E. GREEN¹, YUSONG LIU¹, XINXIN CHENG¹, PHILIPP LENZEN¹, XIAOZHE SHEN¹, ●KASRA AMINI², FERNANDO RODRIGUEZ DIAZ², FABIANO LEVER³, XIAOJUN WANG³, MARKUS GUEHR³, MIKE MINITTI¹, JOEL ENGLAND¹, and ALEXANDER H. REID¹ — ¹SLAC National Accelerator Laboratory, Menlo Park, CA, USA — ²Max-Born-Institut, Max-Born-Straße 2A, 12489, Berlin, Germany — ³Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Molecular photoswitches, exemplified by azobenzene (AB), represent a key class of molecules displaying optical switching and structural rearrangement around a double bond - a process that is fundamental to human vision. Ab initio calculations predict that optical excitation of trans-AB to its second excited state at 297-nm undergoes trans-to-cis isomerization with a quantum yield of 12% within a 350-fs timescale. However, experimental investigations into the photochemistry and nuclear dynamics of gas-phase AB remain limited. Here, we present an ultrafast electron diffraction (UED) study of trans-to-cis isomerization in AB between 267-nm and 330-nm using the MeV-UED instrument at SLAC. We show that the onset of isomerization is wavelength-dependent, and we measure the first direct observation of the transient cis isomer which is formed within the predicted 350-fs timescale.

MO 13.3 Wed 11:30 HS XVI

Semiclassical simulations of laser-induced electron diffraction — ●ÁLVARO FERNÁNDEZ^{1,2}, ANDREY YACHMENEV^{1,3}, and JOCHEN KÜPPER^{1,2,3} — ¹Deutsches Elektronen-Synchrotron, DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg

Laser-induced electron diffraction (LIED) [1] is a tabletop imaging technique capable of measuring photoelectron probability densities, which allow for determining nuclear positions with sub-bondlength and femtosecond precision. In LIED, electrons have much lower energies than those of standard electron diffraction and are significantly perturbed by interactions with the parent ion during rescattering. Consequently, retrieving molecular structures from LIED requires accurate theoretical simulations of the complex photoelectron dynamics.

We present the implementation and results of semiclassical simulations of LIED [2]. In our model, the ionisation step is computed quantum-mechanically using the MO-ADK or Dyson formalisms. Subsequent photoelectron propagation and rescattering are treated classically, modelling the electrostatic potential of the parent ion using chosen quantum-chemical method. To obtain accurate results, billions

of different electron trajectories are simulated. The approach is implemented as a Python package, and its computational performance and accuracy are validated in simulations of OCS and indole-water molecules.

- [1] Karamatskos, E. T., *et al.*, *J. Chem. Phys.*, **150**, 24 (2019)
 [2] Wiese, J., *et al.*, *Phys. Rev. Research*, **3**, 013089, (2021)

MO 13.4 Wed 11:45 HS XVI

Towards Ultrafast Molecular Dynamics in Chiral Molecules in a Micro-solvated Environment — ●LILIANA M. RAMOS MORENO¹, DEEPAK K. PANDEY¹, SAGNIK DAS¹, CLAUS-PETER SCHULZ², HENDRIKE BRAUN-KNIE¹, and JOCHEN MIKOSCH¹ — ¹Institut für Physik, Universität Kassel, Kassel, Germany — ²Max Born Institute (MBI), Berlin, Germany

The environment surrounding a molecule, its solvent, affects the molecular properties and reaction dynamics. Solution in water is of particular relevance in biology and chemistry. Water is also of great fundamental interest as the “universal solvent”, with the ability to dissolve more substances than most other liquids. We follow a bottom-up approach to investigate solution effects with femtosecond laser spectroscopy step-by-step, by adding water molecules one at a time to a small molecule in the gas phase. The clusters are produced in a temperature-variable molecular beam source[1]. The experiments are performed in a Photoelectron Photoion Coincidence (PEPICO) spectrometer. It consists of a magnetic bottle for photoelectrons and a Wiley-McLaren spectrometer for photoions, allowing us to retrieve time-of-flight spectra, in coincidence. We will present our experimental setup and the progress of an experiment where we study the time-dependent Circular Dichroism (CD) in 3-methyl cyclopentanone (3-MCP). The temperature-variable source allows us to change the conformer composition of 3-MCP and test a hypothesis established in recent work[2]. [1]Müller et al., *JPCA* **118**, 8517 (2014) [2]Das et al., Control of circular dichroism in ion yield of 3-methyl cyclopentanone with femtosecond laser pulses(submitted).

MO 13.5 Wed 12:00 HS XVI

Dynamics of pyrrole-water studied by Coulomb-explosion imaging — ●SEBASTIAN TRIPPEL^{1,2} and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Center for Ultrafast Imaging, Universität Hamburg — ³Department of Physics, Universität Hamburg

Microsolvated biomolecules are promising model systems for studying the corresponding light-induced dynamics of molecules in solution [1]. Due to the still manageable complexity of the small clusters in the gas phase, atomic, molecular, and optical physics methods can be used to analyze and characterize their dynamics. Here, we will present our findings on the dynamics of ionized pyrrole-water [2]. Furthermore, we will discuss the creation of highly charged carbon atoms observed for the microsolvated clusters.

- [1] L. He, *et int.* (8 authors), J. Küpper, *J. Phys. Chem. Lett.* **14**, 10499 (2023)
 [1] M. Johny, *et int.* (6 authors), J. Küpper, *Phys. Chem. Chem. Phys.* **26**, 13118 (2024)

MO 13.6 Wed 12:15 HS XVI

Unraveling the dynamics of ionized water dimer in a highly-purified molecular beam — ●IVO S. VINKLÁREK¹, HUBERTUS BROMBERGER¹, LUISA BLUM^{1,2}, SEBASTIAN TRIPPEL¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Physics, Universität Hamburg, Hamburg, DE — ³Center for Ultrafast Imaging, Universität Hamburg, Hamburg, DE

Radiation chemistry in biochemical systems is primarily driven by the ultrafast dynamics of water molecules after absorption of ionizing radiation. The initial water response to the ionization involves ultrafast hydrogen-bond-mediated proton transfer (PT), which was recently probed in the prototypical water-dimer cation (H₂O)₂⁺ [1], and subsequent fragmentation into highly reactant ions and radicals.

Our detailed study utilizing purified molecular beams of (H₂O)₂⁺ [2] revealed that (H₂O)₂⁺ can either stabilize or undergo fragmentation along more than ten distinct pathways. While theoretical studies have explored the rates and dynamics of some of these reactions, experimental evidence is completely lacking. To address this, we employed

a disruptive-probing scheme [3] that allows us to track early PT dynamics and the populations of ionic products, thus directly yielding effective reaction-rate constants. These findings provide crucial insights into ionizing processes in both the atmosphere and living organisms.

- [1] Schnorr, K. *et al.*, *Sci. Adv.* 9, eadg7864 (2023)
- [2] Vinklársek, I.S. *et al.*, *J. Phys. Chem. A* 128, 1593 (2024),
- [3] Jochim, B. *et al.*, *Rev. Sci. Instrum.* 93, 033003 (2022)

MO 13.7 Wed 12:30 HS XVI

Understanding fragmentation dynamics of difluorodiodomethane — ●NIDIN VADASSERY^{1,3}, SEBASTIAN TRIPPEL^{1,2,4}, and JOCHEN KÜPPER^{1,2,3,4} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany — ³Department of Chemistry, Universität Hamburg, Hamburg, Germany — ⁴Department of Physics, Universität Hamburg, Hamburg, Germany

Unimolecular photo-fragmentation is crucial in environmental chemical reactions like ozone depletion and aerosol formation [1]. Photodissociation of polyhalohydrocarbons significantly contributes to these climate-impacting processes. Difluorodiodomethane (CF₂I₂) exhibits unconventional dynamics near dissociative energies [2]. We present experimental results exploring CF₂I₂ dissociation dynamics using near-infrared laser pulses. A pure CF₂I₂ sample was produced using an electrostatic deflector, revealing metastable states and quantum-state-specific dynamics during photo-fragmentation [3]. We also outline a time-resolved x-ray diffraction approach and present computational

results of diffraction simulations for laser-aligned gas-phase CF₂I₂.

- [1] J. C. G. Martin, *et al.*, *J. Am. Chem. Soc.* 144, 9240 (2022)
- [2] P. Z. El-Khoury, *et al.*, *J. Chem. Phys.* 132, 124501 (2010)
- [3] I. S. Vinklársek, *et int.* (3 authors), J. Küpper, S. Trippel, *J. Phys. Chem. A* 128, 1593(2024) *arXiv:2308.08006* [physics].

MO 13.8 Wed 12:45 HS XVI

Single and Double Ionization of Pyridine and Pyridine-water Complexes — ●SITANATH MONDAL¹, BRENDAN WOUTERLOOD¹, MYRIAM DRISSI², GUSTAVO A. GARCIA², LAURENT NAHON², FRANK STIENKEMEIER¹, and SEBASTIAN HARTWEG¹ — ¹Institute of Physics, Albert-Ludwigs-Universität Freiburg, Germany — ²Desirs Beamline, Synchrotron Soleil, St. Aubin, France

Cell and gene damage caused by slow electrons created by secondary processes after interaction with ionizing radiation is an important field of research. Photoelectron studies of biomolecule-water complexes in the gas phase can give us insight about some of the fundamental processes producing low energy secondary electrons and inducing fragmentation of cationic products. I will present a photoelectron photoion coincidence study of pyridine, pyridine clusters, and pyridine-water complexes considering single and double ionization processes. Our data provides insight on the single and double ionization energies of these systems and reveals differences in the dissociation pathways of pyridine in different environments. The ion-ion coincidence spectroscopy allows us to distinguish between different local double ionization and non-local double ionization mechanisms like intermolecular Coulombic Decay.

MO 14: Polaritonic Effects in Molecular Systems II (joint session MO/Q)

Time: Wednesday 11:00–13:00

Location: HS XV

MO 14.1 Wed 11:00 HS XV

Boundary conditions and violations of bulk-edge correspondence in a hydrodynamic model — GIAN MICHELE GRAF¹ and ●ALESSANDRO TARANTOLA^{1,2} — ¹Institut für Theoretische Physik, Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland — ²German Aerospace Center (DLR), Institute of Quantum Technologies, 89081 Ulm, Germany

Bulk-edge correspondence is a wide-ranging principle that applies to topological matter. According to the principle, the distinctive topological properties of matter, thought of as extending indefinitely in space, are equivalently reflected in the excitations running along its boundary. Indices encode those properties, and their values, when differing, are witness to a violation of that correspondence. We address such violations, as they occur in a hydrodynamic context. The model concerns a shallow layer of fluid in a rotating frame and provides a local description of waves propagating either across the oceans or along a coastline; it becomes topological when suitably modified at short distances. The edge index is sensitive to boundary conditions, hence exhibiting a violation. Here we present a classification of all (local, self-adjoint) boundary conditions. They come in four families, distinguished in part by the degree of their underlying differential operators. Generally, both the correspondence and its violation are typical. Across families though, the maximally possible amount of violation can vary with their degree. Several indices of interest are charted for all boundary conditions. A single spectral mechanism for the onset of violations is furthermore identified, and the role of a symmetry investigated.

MO 14.2 Wed 11:15 HS XV

Cavity-mediated electron-electron interactions: Renormalizing Dirac states in graphene — ●HANG LIU¹, FRANCESCO TROISI¹, HANNES HUEBENER¹, SIMONE LATINI^{1,2}, and ANGEL RUBIO^{1,3} — ¹Max Planck Institute for the Structure and Dynamics of Matter, Germany — ²Technical University of Denmark, Denmark — ³The Flatiron Institute, USA

Accurately modeling the interaction between electrons in materials and photon modes within dark cavities is crucial for predicting and understanding cavity-induced phenomena. In this work, we developed the photon-free quantum electrodynamics Hartree-Fock and configuration-interaction frameworks to model the coupling between electrons in crystalline materials and cavity photon modes. We applied these theoretical approaches to investigate the graphene coupled to different types of cavity modes. For a circularly polarized mode, a topological

Dirac gap emerges due to cavity-mediated local and nonlocal electron interactions. In contrast, a linearly polarized mode induces a topologically trivial Dirac gap as a result of the cavity-mediated nonlocal electron interactions. Notably, when two cavity modes are introduced, the Dirac cones can remain gapless, but the Fermi velocity is renormalized through cavity-induced nonlocal electron interactions. Our non-perturbative approaches can capture the critical role of cavity-induced nonlocal electron-electron interactions in renormalizing Dirac states in graphene. These new theoretical frameworks pave the way for accurately predicting and exploring novel cavity-induced phenomena in a broader range of material systems.

MO 14.3 Wed 11:30 HS XV

Quantum algorithms for QED systems — ●FRANCESCO TROISI¹, SIMONE LATINI², HEIKO APPEL¹, IVANO TAVERNELLI⁴, and ANGEL RUBIO^{1,3} — ¹MPSD, Hamburg, Germany — ²Department of Physics, DTU, Lyngby, Denmark — ³CCQ, Flatiron Institute, Simons Foundation, NYC, USA — ⁴IBM Quantum, IBM Research, Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

Controlling the properties of matter is a central theme in modern science. Optical cavities provide a promising approach to controlling them by coupling the electronic transitions to the confined photons inside the cavity, making the photonic and electronic states inseparable. The polaritonic states are obtained, which due to the strong coupling regime, cannot be described by the perturbative approach. On a classical computer, this introduces big computational challenges as the QED matrix grows exponentially with the number of photonic modes and Fock states. Quantum Computing is a promising tool for studying such systems as adding one cavity mode requires as little as one qubit. Due to the complexity of the physics in materials or complex molecules, we approach the cavity QED problem with a simpler system, such that we can learn the challenges in a controlled environment. In this work we couple a two-level matter system to many cavity modes, and we focus on studying a well-known physical phenomenon, the spontaneous emission, where excited atoms emit photons upon returning to their ground state. Despite its simplicity, one can still observe many features such as the Rabi oscillations and the decay rate making it an ideal candidate for approaching QED problems.

MO 14.4 Wed 11:45 HS XV

Control of cavity dissipations across the insulator-to-metal transition in 1T-TaS₂ — ●GIACOMO JARC¹, ANGELA MONTANARO¹, SHAHLA YASMIN MATHENGATTIL^{2,3}, ENRICO

RIGONI^{1,3}, and DANIELE FAUSTI¹ — ¹Department of Physics, FAU Erlangen-Nürnberg Erlangen, Germany — ²Department of Physics, Università di Trieste, Trieste, Italy — ³Elettra Sincrotrone, Basovizza (Trieste), Italy

Using optical cavities resonant with material excitations enables controlling light-matter interaction in both the regimes of weak and strong coupling. We study here the coupling of low-energy excitations in the charge-density-wave (CDW) material 1T-TaS₂ across its insulator-to-metal transition when embedded into tetrahertz Fabry-Pérot cryogenic cavities. In the dielectric state, we reveal the signatures of a multimode vibro-polariton mixing, with the polariton modes inheriting character from all the CDW phonons as a consequence of the cavity-mediated hybridization. The multimode vibrational strong coupling is suppressed across the insulator-to-metal transition as a consequence of the optical dissipations introduced by the free charges, and a vibrational weak coupling regime is observed in proximity of the phase transition. When the cavity frequency is tuned within the spectral range of the continuum Drude excitation, we reveal that the quality factor of the cavity, which quantifies the dissipations of the coupled system, decreases passing from the insulating to the metallic state. Our evidences points to a scenario in which the free charges can effectively couple to the cavity field and subsequently modify the collective light-matter coupling.

MO 14.5 Wed 12:00 HS XV

Chirality and Dimensionality in the Ultrastrong Light-matter Coupling Regime — ●RÉMI AVRILLER¹ and CYRIAQUE GENET² — ¹University of Bordeaux, CNRS, LOMA, UMR 5798, F-33405 Talence, France. — ²University of Strasbourg and CNRS, CESQ and ISIS, UMR 7006, F-67000 Strasbourg, France

We unveil the key-role of dimensionality in describing chiroptical properties of molecules embedded inside an optical Fabry-Pérot cavity.

For a 2D-layer configuration, we show that the interplay between molecular chirality and spatial dispersion of the cavity-modes, results in a gyrotropic coupling at the origin of a differential shift in polaritonic energy spectra. This differential shift is proportional to the gyrotropic coupling, while for 3D bulk-aggregate configurations it is shown to vanish.

We interpret physically the former 2D-chiral effect by analogy with the classical Newtonian motion of a fictitious particle in presence of 3D restoring force, and static magnetic field. The gyrotropic coupling is shown to directly perturbate the anholonomy angle of the classical trajectories, and the fictitious particle undergoes cyclotron gyrations upon entering the ultrastrong light-matter coupling regime.

MO 14.6 Wed 12:15 HS XV

The complex interplay of collectivity, locality and temperature in polaritonic chemistry — ●DOMINIK SIDLER^{1,2,3}, MICHAEL RUGGENTHALER^{2,3}, JACOB HORAK^{2,3}, THOMAS SCHNAPPINGER⁴, and ANGEL RUBIO^{2,3,5} — ¹Paul Scherrer Institut, Villigen, Switzerland — ²Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ³The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — ⁴Stockholm University, Stockholm, Sweden — ⁵The Flatiron Institute, New York, USA

Despite significant theoretical progress over the past years, still, no consensus has been achieved about the physically relevant mechanism in polaritonic chemistry. Based on ab initio simulations and analytic results, we will explore and identify physical mechanisms that shine light on the interplay of collective strong coupling with local chemical

changes. For its detailed microscopic understanding, degeneracies and cavity-induced local polarization patterns seem to play a crucial role. To capture those effects accurately, a fully self-consistent description is vital, since perturbation theory can lead to qualitatively erroneous predictions. Eventually, we demonstrate that the thermal statistic is altered non-trivially by collective strong coupling in optical cavities. Therefore, novel computational methods are required to simulate polaritonic chemistry accurately.

MO 14.7 Wed 12:30 HS XV

Controlling Plasmonic Catalysis via Strong Coupling with Electromagnetic Resonators — JAKUB FOJT, PAUL ERHART, and ●CHRISTIAN SCHÄFER — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Plasmonic excitations decay within femtoseconds, leaving nonthermal (often referred to as *hot*) charge carriers behind that can be injected into molecular structures to trigger chemical reactions that are otherwise out of reach - a process known as plasmonic catalysis. In this talk, we demonstrate that strong coupling between resonator structures and plasmonic nanoparticles can be used to control the spectral overlap between the plasmonic excitation energy and the charge injection energy into nearby molecules. Our atomistic description couples real-time density-functional theory self-consistently to an electromagnetic resonator structure via the radiation-reaction potential [1,2]. Control over the resonator provides then an additional knob for nonintrusively enhancing plasmonic catalysis [3], here more than 6-fold, and dynamically reacting to deterioration of the catalyst - a new facet of modern catalysis.

[1] C. Schäfer and G. Johansson, PRL 128, 156402 (2022). [2] C. Schäfer, J. Phys. Chem. Lett. 2022, 13, 6905-6911. [3] J. Fojt, P. Erhart, C. Schäfer, Nano Lett. 2024, 24, 11913-11920.

MO 14.8 Wed 12:45 HS XV

Role of Symmetry in Charge Transfer Complexation under Vibrational Strong Coupling — ●ANJALI JAYACHANDRAN, CYRIAQUE GENET, and THOMAS EBBESEN — University of Strasbourg, CNRS, ISIS and icFRC, 8 Allée Gaspard Monge, 67000 Strasbourg, France

The relation between symmetry and chemical reactivity has been explored for a long time. We reported earlier that symmetry also plays a key role in charge transfer (CT) complexation reactions under vibrational strong coupling (VSC) (1). We have now extended this study to a variety of donors and acceptors to gain further insight into how symmetry is acting on VSC. The experiments were conducted using the three isomers of trimethylbenzene (methyl groups in the 1,3,5; 1,2,4 and 1,2,3 positions on the benzene ring) as the donors with acceptors such as iodine, chloranil and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone. It is observed that under vibrational strong coupling, there are large changes in the equilibrium constant, coefficient of absorption and the thermodynamic parameters for the different isomers. The changes seen in these parameters are dependent on the symmetry of the vibrational mode that is coupled to the IR cavity modes as well as the overall symmetry of the molecule. The result of this study confirms the relevance of symmetry in chemical reactivity under VSC and should be taken into consideration to steer reactions towards a desired outcome in this regime. 1. Y. Pang, A. Thomas, K. Nagarajan, R. M. A. Vergauwe, K. Joseph, B. Patrahau, K. Wang, C. Genet, T. W. Ebbesen, Angew. Chem. Int. Ed. 2020, 59, 10436.

MO 15: Interaction with VUV and X-ray Light I (joint session A/MO)

Time: Wednesday 11:00–12:45

Location: GrHS Mathe

MO 15.1 Wed 11:00 GrHS Mathe

High-resolution photoelectron spectroscopy with broad bandwidth pulses from high-harmonic sources — ●SARANG DEV GANESHAMANDIRAM¹, TOBIAS WITTING², ULRICH BANGERT¹, DANIEL UHL¹, LAUREN DRESCHER², BENJAMIN MAINGOT², OLEG KORNILOV², FRANK STIENKEMEIER¹, MARC J.J. VRAKING², and LUKAS BRUDER¹ — ¹Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — ²Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

Extreme ultraviolet time-resolved photoelectron spectroscopy (XUV-TRPES) is a promising emerging method to study molecular dynamics.

However, XUV pulses generated by high harmonic generation (HHG) exhibit very broad spectra, which leads to low spectral resolution in PES experiments, especially involving molecules.

Here, we explore a new approach of Fourier-Transform (FT) based XUV-PES that provides high spectral resolution, while temporal resolution is retained. This approach avoids the photon broadening problem and can disentangle the photoelectrons produced by different harmonics within the HHG spectrum. As model systems serve Rb atoms, and N₂ and O₂ molecules.

MO 15.2 Wed 11:15 GrHS Mathe

Coherent control of strongly driven quantum dynamics us-

ing shaped extreme ultraviolet pulses — ●LUKAS BRUDER — Institute of Physics, University of Freiburg, Germany

The shaping of femtosecond light fields with pulse shapers is a powerful technique enabling the control of quantum dynamics with high selectivity. While the technique is well established in the visible to infrared domain, comparable methods do not exist at shorter wavelengths in the XUV or X-ray domain. We have recently demonstrated the first coherent control experiment using pulse shaping in the XUV domain [1]. We show high fidelity quantum control of Rabi dynamics in helium atoms. In particular, the selective suppression of the two-photon ionization rate could be demonstrated and the strong dressing of continuum states was revealed, which is otherwise difficult to access at long wavelengths.

The results originate from the joint effort of many international laboratories and of a large number of researchers[1], whose work is gratefully acknowledged.

[1] F. Richter et al., arXiv:2403.01835 (2024)

MO 15.3 Wed 11:30 GrHS Mathe

Exceptional points at x-ray wavelengths — ●FABIAN RICHTER¹, LARS BOCKLAGE², RALF RÖHLSBERGER², XIANGJIN KONG³, and ADRIANA PÁLFFY¹ — ¹Julius-Maximilians-Universität Würzburg — ²Deutsches Elektronen Synchrotron DESY, Hamburg — ³Fudan University, Shanghai

Non-Hermitian Hamiltonians effectively describe dissipative systems, exhibiting phenomena absent in the Hermitian realm. Exceptional Points (EPs) are a prime example of this. At EPs not only the complex eigenvalues, but also the eigenvectors coalesce and sensitivity to perturbations is drastically enhanced. This concept has recently advanced in optics, where non-Hermitian eigenstates arise through optical gain and loss [1]. So far, these concepts have been mostly discussed in the optical regime. Similar control of x-rays is desirable due to their superior penetration power, high focusability and detection efficiency.

Here, we investigate non-Hermitian x-ray photonics in thin-film cavities with Mössbauer nuclei under grazing-incidence x-ray radiation. These cavities present loss that can be controlled via adjustment of the cavity geometry and the incidence angle of the x-rays [2]. The application of a magnetic hyperfine field enables tuning the system towards EPs. We theoretically determine the magnetic field strength at which an EP occurs and predict qualitatively distinct behavior in the time spectrum at higher and lower field strengths. Analysis of experimental data confirms these predictions.

[1] L. Feng et al., Nature Photon. 11, 752-762 (2017).

[2] J. Evers, K. P. Heeg, Phys. Rev. A 88, 043828 (2013).

MO 15.4 Wed 11:45 GrHS Mathe

Superradiant Parametric Mössbauer Radiation Source — ●ZHE-AN PENG, CHRISTOPH H. KEITEL, and JÖRG EVERS — Max Planck Institute for Nuclear Physics, Heidelberg, Germany

Mössbauer nuclei facilitate a broad range of applications due to their extremely narrow resonance at x-ray frequency. However, it also renders a strong excitation via x-rays challenging. Here, we propose to construct a superradiant parametric Mössbauer radiation source, which is based on coherently modulated electron bunches exiting from x-ray free-electron laser (XFEL) undulator and passing through a crystal containing Mössbauer isotopes. Due to the constructive interference between the virtual-photon fields of different electrons in a single XFEL electron bunch, the intensity of Mössbauer radiation generated from the crystal can be boosted superradiantly, which scales with the square of electron number of XFEL electron bunch. This tremendous superradiant boost of Mössbauer radiation is also realized by a new geometry we proposed, which can be optimized by experimentally simple ways. Our study bears potential to enable coherent Mössbauer pump-probe spectroscopy, as well as nonlinear Mössbauer optical effects triggered by coherent XFEL electron beam.

[1] O. D. Skoromnik, I. D. Feranchuk, J. Evers, and C. H. Keitel, Phys. Rev. Accel. Beams 25, 040704 (2022).

MO 15.5 Wed 12:00 GrHS Mathe

Single-shot electron spectroscopy of highly transient matter — ●SARA SAVIO¹, LARS FUNKE¹, NICLAS WIELAND², THORSTEN OTTO³, LASSE WUELFING¹, MARKUS ILCHEN^{2,3}, and WOLFRAM HELML¹ — ¹Technische Universität — ²University of Hamburg — ³Deutsches Elektronen-Synchrotron

Core-level photoionization is the process of absorbing a photon by an atom or molecule, ejecting an electron from one of its inner shells and creating a vacancy. This vacancy is then filled through various relaxation processes, which can lead to the emission of secondary electrons or energy redistribution within the system. We explore the generation of double-core holes (DCH) in gaseous neon atoms, which have a very short lifetime, using intense and ultrashort pulses on the attosecond scale at the European XFEL. The ultrafast electron dynamics are mapped on a single-shot basis using an electron time-of-flight (eTOF) spectrometer. Non-invasive systematic pulse characterization using the angular streaking technique provides spectral and temporal information about the ionizing XFEL pulses with attosecond resolution. We conduct a comprehensive study of how the contribution of DCH channels varies with beam parameters, including pulse duration, pulse energy, and the centres of the reconstructed spectra. Examining the electronic structure of the core-ionized system before relaxation, combined with the detailed information about the ionizing pulse, provides valuable insights into the nonlinear photoabsorption and the ultrafast process at extreme intensities on the time scales of electron dynamics.

MO 15.6 Wed 12:15 GrHS Mathe

Cavity-controlled X-ray emission spectra — ●SHU-XING WANG^{1,2}, XIN-CHAO HUANG³, ZHE-QIAN ZHAO⁴, XI-YUAN WANG⁴, and LIN-FAN ZHU⁴ — ¹I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany — ²Helmholtz Forschungszentrum für Schwerkraftforschung, Campus Gießen, 35392 Giessen, Germany — ³FXE instrument, European XFEL, Schenefeld 22869, Germany — ⁴University of Science and Technology of China, Hefei, 230026, China

We report on the X-ray emission spectra from a thin-film cavity sample, measured using a von Hamos spectrometer at the GALAXIES beamline of the SOLEIL synchrotron radiation facility in Paris. The cavity consists of a multilayer structure: 21.8 nm Pt / 203.3 nm C / 29.4 nm WSi₂ / 201.0 nm C / 144.6 nm Pt, deposited on a silicon substrate. X-ray emission spectra covering the L α emission lines of W were recorded by scanning the incident X-ray energy across 10160-10240 eV (L₃ edge of W) at grazing angles near the first cavity mode. Our measurements reveal the collective Lamb shift and superradiant enhancement associated with the inner-shell transition. Notably, by concentrating on the resonant X-ray emission channel, we suppress the influence of the absorption edge, which might otherwise obscure the observed quantum optical effects.

MO 15.7 Wed 12:30 GrHS Mathe

Measurement of resonant nuclear phase shift with a double-waveguide nano-interferometer — ●LEON MERTEN LOHSE^{1,2,3}, RALF RÖHLSBERGER^{4,5,6,1,3}, and TIM SALDITT² — ¹The Hamburg Centre for Ultrafast Imaging, Hamburg — ²Georg-August-Universität Göttingen — ³Deutsches Elektronen-Synchrotron DESY, Hamburg — ⁴Friedrich-Schiller-Universität Jena — ⁵Helmholtz-Institut Jena — ⁶GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt

The phase of an electromagnetic wave is shifted upon scattering off atoms, coherently accumulating to result in the macroscopic index of refraction. In optical waveguides, propagating photons are spatially confined and can be coupled to resonant atoms in a controllable way. We interferometrically measured the phase shift that an ultrathin layer of ⁵⁷Fe Mössbauer nuclei coherently imprints onto x-ray photons propagating through a single-mode x-ray waveguide. Using the extracted phase shift, we were able to accurately quantify the coupling strength between individual photons and nuclei. Based on this, one can envision to actively control the phase in nanophotonic devices.

MO 16: In Memoriam of Hermann Haken (joint session Q/MO)

Physicist Hermann Haken, who died on August 14, 2024 at the age of 97, made groundbreaking contributions to solid-state physics and quantum optics. As a pioneer of laser theory, he recognized early on the ubiquity of non-equilibrium phase transitions. This led to the foundation of the self-organization theory of synergetics, which has been applied to countless systems of both inanimate and living nature. The Symposium honours his life work and outlines exemplarily how his scientific achievements live on in current quantum optics research.

Time: Wednesday 11:00–13:00

Location: HS I PI

Invited Talk MO 16.1 Wed 11:00 HS I PI
Haken's quantum field theoretical understanding of semiconductors and lasers and its present-day impact — ●CUN-ZHENG NING — Shenzhen Technology University, China

Prof. Haken was among the earliest few who applied the then-new quantum field theory (QFT) to understand physical processes in semiconductors in the 1950s and lasers in the 1960s. The first decade of his scientific career was devoted to the QFT treatment of non-metallic solids. His long-lasting impacts are reflected by popular terms such as the Haken Potential for excitons and Feynman-Haken Path Integral for calculating the ground-state energy of polarons. The second decade of his career started at Stuttgart. It was devoted to the newly invented laser whose fundamental understanding, as he quickly realized, required extending the known QFT to include noise and dissipation. In the process, he established the full quantum theory for open systems and laid the foundation for Synergetics. His laser theory not only explained or predicted many phenomena in lasers but also provided a general framework for the understanding of problems whenever light-matter interaction is involved. While his first two decades focused on the QFT treatment of semiconductors or light field respectively, a proper description of semiconductor optics requires the QFT treatment of both semiconductors and optical field self-consistently. This task turns out to be as challenging as it is rewarding when Coulomb interaction is included and remains an active field of research today, continued by generations of his students. This talk will cover aspects of Prof Haken's early contributions and some recent progress.

Invited Talk MO 16.2 Wed 11:30 HS I PI
Bose-Einstein condensation of photons in vertical-cavity surface-emitting lasers — ●MACIEJ PIECZARKA — Wrocław University of Science and Technology, Wrocław, Poland

Professor Haken pioneered the development of the quantum theory of lasers and discovered that lasing action can be viewed as a nonequilibrium second-order phase transition. This visionary and broader view inspired many to find a link between lasing and the Bose-Einstein condensation (BEC) of photons. It appears that the worlds of lasers and BEC are deeply intertwined, as BEC was found in dye-filled microcavities [1] and, more recently, in semiconductor lasers [2].

I will present our demonstration of photon BEC phase transition in a real-world device - a Vertical-Cavity Surface-Emitting Laser (VCSEL) [2]. Besides distinctive differences from the complete thermal equilibrium, we show that photons in a VCSEL follow the equation of state for an ideal bosonic gas. We argue that photon BEC can be a much more common phenomenon in laser physics than previously anticipated.

[1] J. Klaers et al., *Nature* **468**, 545 (2010).

[2] M. Pieczarka et al., *Nature Photonics* **18**, 1090 (2024).

Invited Talk MO 16.3 Wed 12:00 HS I PI
Photons in a dye-filled cavity: quantum-optical system interpolating between Bose-Einstein condensates and laser-like states — ●MILAN RADONJIĆ — Universität Hamburg, Germany — University of Belgrade, Serbia

It is well known that photons in a dye-filled cavity exhibit a Bose-Einstein condensate (BEC) of light [1]. We generalize the microscopic non-equilibrium Kirtton-Keeling model [2] of such a system by carefully considering the interplay of coherent and dissipative dynamics within the Lindblad master equation framework pioneered by Hermann Haken in his theory of lasers [3]. The resulting equations of motion of both photonic and matter degrees of freedom are then used to study the steady-state properties of the system. We demonstrate that this system can interpolate between photon BEC and laser-like states, depending on whether the dissipative or coherent influence of the environment is dominant [4]. In the former case, we show that the cavity modes of different energies are essentially uncorrelated. In the laser-like regime, some cavity mode acquires macroscopic occupation, while the populations of other cavity levels strongly deviate from the Bose-Einstein distribution. Additionally, the steady state contains a rather high degree of correlations between the different cavity modes.

[1] J. Klaers et al., *Nature* **468**, 545 (2010).

[2] P. Kirtton and J. Keeling, *Phys. Rev. Lett.* **111**, 100404 (2013).

[3] H. Haken, *Laser Theory*, Springer (1970, 1984).

[4] M. Radonjić et al., *New J. Phys.* **20**, 055014 (2018).

Invited Talk MO 16.4 Wed 12:30 HS I PI
From laser physics to nonlinear dynamics and synergetics — ●ECKEHARD SCHÖLL — TU Berlin, Germany

Hermann Haken was a pioneer of laser physics and developed the first full quantum theory of the laser [1]. He interpreted the laser transition as a nonequilibrium phase transition [2], and found that this is a special case of a much wider class of open systems driven far from thermodynamic equilibrium. Based upon this observation he founded the field of synergetics which deals with systems composed of many subsystems like atoms, molecules, photons, cells, etc., and shows that cooperation of the subsystems leads to spatial, temporal, or functional structures by self-organization [3]. He demonstrated that the semiclassical laser equations are mathematically equivalent to the Lorenz equation derived from fluid dynamics [4], exhibiting higher instabilities and chaos, like many other nonlinear dynamical systems in physics, chemistry, biology, medicine, and even economics, sociology and psychology. This has given rise to a plethora of new phenomena in nonequilibrium system widely studied during the past five decades. Coherence resonance is just one example which was first discovered by Haken [5], and later studied in various systems ranging from lasers to the brain.

[1] H. Haken, *Laser Theory*, Springer (1970, 1984).

[2] R. Graham and H. Haken, *Z. Phys.* **237**, 31 (1970).

[3] H. Haken, *Synergetics, An Introduction*, Springer (1977).

[4] H. Haken, *Phys. Lett.* **53A**, 77 (1975).

[5] G. Hu et al., *Phys. Rev. Lett.* **71**, 807 (1993).

MO 17: Members' Assembly

Time: Wednesday 13:15–14:15

Location: HS 5

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

MO 18: Cold Molecules and Cold Chemistry (joint session MO/Q)

Time: Wednesday 14:30–16:30

Location: HS XVI

Invited Talk

MO 18.1 Wed 14:30 HS XVI

Cold and Controlled Reactive Collisions — ●JOLIIN ONVLEE — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

What exactly happens during a chemical reaction? Our aim is to investigate fundamental chemical reactions and their underlying dynamics at the full quantum level. To achieve this, we let individual molecules and atoms collide and react with each other in a crossed molecular beam machine.

We can precisely control the velocity and quantum state of a paramagnetic reactant before the collision by using a Zeeman decelerator. After the collision, we accurately probe the reaction products and their velocity vectors using laser-based techniques and velocity map imaging. This powerful combination of techniques allows for scattering experiments with extraordinary resolution.

Here, I will show how we use this approach to investigate the prototypical insertion reaction between excited sulfur atoms and hydrogen molecules in high detail and in unexplored energy regimes. With these experiments, we aim to provide a sensitive test for potential energy surfaces and scattering calculations used to describe the molecular reaction dynamics in this system. This will enable us to deepen our understanding of the intricate dynamics underlying a reaction.

MO 18.2 Wed 15:00 HS XVI

Low-energy collisions between two indistinguishable tritium-bearing hydrogen molecules: HT+HT and DT+DT — ●RENAT SULTANOV — The University of Texas Permian Basin, Odessa, Texas, USA

Elastic and rotational energy transfer collisions between two tritium-containing hydrogen molecules are computed at low- and very low energies, down to ultra-cold temperatures: $T \simeq 10^{-8}$ K. A pure quantum-mechanical approach is applied. A high-quality global six-dimensional potential energy surface (PES) has been appropriately modified and used in these calculations. In the case of the symmetrical $H_2 + H_2$ or $D_2 + D_2$ collisions one can use the original H_4 PES as it is, i.e. without transformations. However, in the case of the non-symmetrical (or symmetry-broken) $HD + H_2/D_2$, $HT + HT$, $DT + DT$ scattering systems one should also apply the original H_4 potential (PES), but propagation (solution) of the Schrödinger equation runs (in this case) over the corrected Jacobi vector [1,2]. Elastic and state-selected inelastic cross sections and corresponding thermal rate coefficients will be presented.

1. R. A. Sultanov, D. Guster, S. K. Adhikari, Phys. Rev. A 85, 052702 (2012).

2. R. A. Sultanov, D. Guster, S. K. Adhikari, J. Phys. B 49 (2016) 015203.

MO 18.3 Wed 15:15 HS XVI

Dual-color microwave-dressing for collisional control in molecular dipolar Fermi gases — ●SEBASTIAN EPELT^{1,2}, SHRESTHA BISWAS^{1,2}, CHRISTINE FRANK^{1,2}, XING-YAN CHEN⁴, WEIKUN TIAN^{1,2}, IMMANUEL BLOCH^{1,2,3}, and XIN-YU LUO^{1,2} — ¹Max-Planck-Institute of Quantum Optics — ²Munich Center for Quantum Science and Technology — ³Ludwig-Maximilians-Universität — ⁴Princeton University

Ultracold polar molecules are a promising platform for the exploration of exotic quantum matter, including topological dipolar p-wave superfluids, thanks to their long-range dipolar interactions. In this talk, we will present our work on microwave-dressing of fermionic $^{23}\text{Na}^{40}\text{K}$ molecules. Using a single, circularly-polarized, blue-detuned microwave field we can engineer intermolecular potential, where inelastic and elastic scattering tuneable via field-linked scattering resonance. This resonance is universal for systems with dipolar interactions and arises due to existence of a stable tetraatomic bound state which we recently observed and characterized in our experiment. Adding a second, linearly polarized microwave field at a different frequency enables control of the long-range dipolar interaction by tuning the dipole-dipole scattering length. This improves our toolbox for creating ultracold, deeply-degenerate samples of dipolar fermionic molecules, necessary in our quest towards realizing a dipolar p-wave superfluid and beneficial for quantum simulations in optical lattices.

MO 18.4 Wed 15:30 HS XVI

Photoassociation Spectroscopy of RbYb near the Yb intercombination line — ●ARNE KALLWEIT — Uni 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 first experiments in our apparatus for the production of ultracold RbYb molecules. This setup constitutes an improvement of our old apparatus, where the interactions in RbYb and possible routes to molecule production have already been studied extensively. In the new setup a major goal is the efficient production of ground state RbYb molecules. We employ optical tweezers to transport individually cooled samples of Rb and Yb from their separate production chambers to a dedicated science chamber. Here we start to study interspecies interactions of different isotopes by overlapping crossed optical dipole traps. To explore the pathways towards ground state molecules we start with photoassociation spectroscopy near the intercombination line of Yb.

MO 18.5 Wed 15:45 HS XVI

Delta-Kick Collimation of Heteronuclear Feshbach Molecules — ●TIMOTHÉ ESTRAMPES^{1,2}, JOSE P. D'INCAO^{3,4}, JASON. R. WILLIAMS⁵, ÉRIC CHARRON², and NACEUR GAALLOUL¹ — ¹Leibniz University Hannover, Institut für Quantenoptik, Germany — ²Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, France — ³JILA, NIST, and the Department of Physics, University of Colorado, Boulder, CO 80309, USA — ⁴Department of Physics, University of Massachusetts Boston, Boston, MA 02125, USA — ⁵Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA

Delta-Kick Collimation [Phys. Rev. Lett. 78, 2088 (1997)] is a well-known process in atomic physics that allows to drastically reduce the expansion energy of a cold sample by flashing an external potential during its release. Here, we theoretically explore the extension of this process to cold heteronuclear Feshbach molecules.

We first investigate the validity of neglecting the coupling between the center-of-mass motion and molecular vibrations. After establishing the domain of validity for this approximation, we use scaling approaches to estimate the achievable gains over a large range of temperature and density regimes. For typical external trap parameters, the expansion energy of a thermal cloud could be reduced by a factor of 100, increasing to over 500 for a heteronuclear condensed molecule.

MO 18.6 Wed 16:00 HS XVI

Laser cooling of barium monofluoride molecules — ●MARIAN ROCKENHÄUSER¹, FELIX KOGEL², TATSAM GARG¹, JAKOB WEISS¹ und TIM LANGEN¹ — ¹TU Wien, Atominstitut, Cold Molecules and Quantum Technologies — ²Universität Stuttgart, 5. Physikalisches Institut

Barium monofluoride (BaF) molecules are sensitive probes for precision tests of fundamental symmetries. However, due to the high mass, comparatively narrow linewidth, resolved hyperfine structure, and potential branching losses through an intermediate electronic state, this molecular species is notoriously difficult to cool. We will report on the observation of Sisyphus-type forces in transversal cooling of ^{138}BaF and the less abundant bosonic isotopologue ^{136}BaF realizing the first isotopologue-selective laser cooling of molecules. Furthermore, we will discuss our progress towards cooling of the fermionic isotopologue ^{137}BaF which involves optical cycling in a 112 level system. Our results are an important step towards using intense beams of barium monofluoride for precision measurement applications, including searches for the electron's electric dipole moment and nuclear anapole moments. We also expect the results to be useful for cooling other molecular species with complex level structure.

MO 18.7 Wed 16:15 HS XVI

High-flux cold lithium-6 and rubidium-87 atoms from compact two-dimensional magneto-optical trap — ●ANWEI ZHU^{1,2}, YUNXUAN LU^{1,2}, XINYI HUANG^{1,2}, CHENHAO NI^{1,2}, and XINYU LUO^{1,3} — ¹Max Planck Institute of Quantum Optics — ²Ludwig Maximilian University of Munich — ³Munich Center for Quantum Science and Technology

We report the development of a compact setup for producing Fermi gas of ultracold ${}^6\text{Li}{}^{87}\text{Rb}$ molecules, which integrates two 2D magneto-optical traps in series for each species with a short-distance lithium Zeeman slower. The Zeeman slower enhances the lithium flux by a factor of 50, achieving a high flux of 1×10^{10} atoms/s at a moderate oven temperature of 370 degrees. In addition, the rubidium flux

reaches a value of 6×10^8 atoms/s. This advancement paves the way for the rapid production of double-degenerate lithium-rubidium atomic mixtures and large samples of ultracold ground-state fermionic lithium-rubidium molecules, providing a robust platform for investigating dipolar interaction and phase transition in ultracold regime.

MO 19: Interaction with Strong or Short Laser Pulses I (joint session A/MO)

Time: Wednesday 14:30–16:15

Location: GrHS Mathe

Invited Talk

MO 19.1 Wed 14:30 GrHS Mathe
Time Resolved Diffractive Imaging of Laser Induced Dynamics in Materials — ●TOM BÖTTCHER, RICHARD ALTENKIRCH, STEFAN LOCHBRUNNER, CHRISTIAN PELTZ, THOMAS FENNEL, and FRANZISKA FENNEL — Institute of Physics and Department of Life, Light and Matter, University of Rostock, 18051 Rostock, Germany

Micromachining with ultrashort laser pulses is widely used for industrial applications. In contrast to picosecond and nanosecond lasers, ultrashort laser pulses allow precise material modifications due to local electronic excitation on timescales well below electron-ion equilibration times and thermal dissipation. However, the underlying processes leading to target modification and ablation after ultrashort laser pulse excitation are still insufficiently understood.

We present an experimental method to study the excitation and relaxation processes in thin gold films using femtosecond to nanosecond single-shot pump probe coherent diffractive imaging. The target is a 30 nm-thick, free-standing gold foil, which is excited using an 800 nm femtosecond pump pulse. The dynamics in the excited foil are imaged after a variable time delay using a 400 nm femtosecond probe pulse which creates a diffraction image that is captured by a CMOS camera. A phase retrieval algorithm is used to reconstruct the 2D spatial and time resolved exit field at the target position from the captured diffraction images. Dynamics are monitored up to 2 ns, providing access to ultrafast excitation (fs-ps regime) as well as melting and ablation dynamics (ps-ns regime).

MO 19.2 Wed 15:00 GrHS Mathe
Ionization and Fragmentation of Polyatomic Molecules in Intense Laser Fields using a Reaction Microscope — ●MARTIN GARRO, NARAYAN KUNDU, HORST ROTTKE, ARNE SENFTLEBEN, and JOCHEN MIKOSCH — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

As attosecond science advances into the study of polyatomic molecules, the many-electron and non-adiabatic phenomena in strong-field ionization (SFI) become relevant. A fundamental question concerns the population of electronically excited states of the cation in the intense field, in particular whether these processes are direct or sequential. We study ionization and fragmentation of polyatomic molecules in intense laser fields experimentally with a Reaction Microscope. Coincidence detection of electron and ion momenta reveal detailed insights into the underlying physics. This presentation highlights our recent work on SFI of 1,3-butadiene, n-butane, and 1-butene, in which the intensities and wavelengths were varied. We observe qualitative changes of experimental observables as a function of these parameters, which we interpret as transition between non-sequential and sequential excitation processes.

MO 19.3 Wed 15:15 GrHS Mathe
Machine learning for retrieval of the time-dependent internuclear distance in a molecule from photoelectron momentum distributions: fully quantum mechanical approach — ●NIKOLAY SHVETSOV-SHILOVSKI and MANFRED LEIN — Leibniz Universität Hannover

We use a neural network for retrieval of the time-varying bond length in a dissociating one-dimensional H_2^+ molecule based on photoelectron momentum distributions (PMDs) from strong-field ionization. In contrast to our previous study [1], the motion of the atomic nuclei is treated fully quantum mechanically, i.e., PMDs are obtained from the solution of the time-dependent Schrödinger equation for the wavefunction depending on both the electron coordinate and the internuclear distance. We show that the neural network can recognize the time-dependent bond length with a good accuracy. Therefore, machine learning can be applied for time-resolved molecular imaging.

[1] N. I. Shvetsov-Shilovski and M. Lein, J. Phys. B: At. Mol. Opt. Phys. 57, 06LT01 (2024).

MO 19.4 Wed 15:30 GrHS Mathe
Harmonic generation with topological edge states and electron-electron interaction — ●SIAMAK POOYAN and DIETER BAUER — Institute of Physics, Rostock University, 18051 Rostock, Germany

It has been found previously that the presence or absence of topological edge states in the Su-Schrieffer-Heeger (SSH) model has a huge impact on harmonic generation spectra. More specifically, the yield of harmonics for harmonic orders that correspond to photon energies below the band gap is many orders of magnitude different in the trivial and topological phase. It is shown in this work that this effect is still present if electron-electron interaction is taken into account, i.e., if a Hubbard term is added to the SSH Hamiltonian. To that end, finite SSH-Hubbard chains at half filling are considered that are short enough to be accessible to exact diagonalization but already showing edge states in the topological phase. We show that the huge difference in the harmonic yield between the trivial and the topological phase can be reproduced with few-level models employing only the many-body ground state and a few excited many-body states.

MO 19.5 Wed 15:45 GrHS Mathe
High-harmonic generation in weakly coupled organic molecular systems — ●FALK-ERIK WIECHMANN^{1,2}, SAMUEL SCHÖPA¹, LINA MARIE BIELKE¹, FELIPE MORALES³, SERGUEI PATCHKOVSKII³, MARIA RICHTER³, DIETER BAUER¹, and FRANZISKA FENNEL^{1,2} — ¹Institute of physics, University of Rostock, 18059 Rostock, Germany — ²Department of Life, Light and Matter, University of Rostock, 18059 Rostock — ³Max Born Institute (MBI) for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

We introduce organic molecular crystals (OMCs) as a novel target class for high-harmonic Generation (HHG), bridging the gap between gas phase and solid state high-harmonic spectroscopy. In OMCs, neighboring molecules experience a weak van-der-Waals coupling, considerably smaller compared to the covalent or ionic bonds in previous solid-state target. However, this finite coupling leads to *solid like* features, e.g. a delocalization of the electronic states over several unit cells. Additionally, the perfect inherent alignment of all molecules makes OMCs an ideal target class for HH 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 0.67 TW/cm² we demonstrate that HHG from Pentacene crystals is possible without imposing physical damage. We find that the harmonic-generation process is driven by collective intermolecular effects and not by the response of non-interacting aligned molecules.

MO 19.6 Wed 16:00 GrHS Mathe
A theoretical perspective on high-harmonic generation in organic molecular crystals — ●SAMUEL SCHÖPA¹, LINA BIELKE¹, FALK-ERIK WIECHMANN¹, FELIPE MORALES², SERGUEI PATCHKOVSKII², MARIA RICHTER², FRANZISKA FENNEL¹, and DIETER BAUER¹ — ¹Institute of physics, University of Rostock, 18059 Rostock — ²Max Born Institute (MBI) for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin

We investigate the underlying mechanism of high-harmonic generation (HHG) in the novel target class of organic molecular crystals (OMCs). Compared to covalent and ionic-bonded solids, the molecules that bond to form OMCs are much more weakly coupled, which is reflected in an energy band structure dominated by single-molecule excitations and charge-transfer states of neighbouring molecules. But does the intramolecular response of the aligned molecules dominate the HHG

process? Or can we exploit HH spectroscopy to study the solid-state properties of OMCs, which are characterized by the intermolecular couplings? We addressed this by simulating the HHG process using full time-dependent density-functional theory (TD-DFT) for different polarizations of the driving field and compared it with experimental results. We find in both, that the rotation of the driver polariza-

tion reveals maxima in the harmonic yield when the polarization is aligned with the axes connecting neighbouring molecules. A simple tight-binding model shows, that lower harmonic orders are primarily governed by the intramolecular response, while higher orders depend mainly on the intermolecular coupling.

MO 20: Poster – Molecular Spectroscopy and Dynamics

Time: Wednesday 17:00–19:00

Location: Tent

MO 20.1 Wed 17:00 Tent

Auger electron spectroscopy of isothiocyanic acid, HNCS — ●DOROTHEE SCHAFFNER¹, MARIUS GERLACH¹, EMIL KARAEV¹, JOHN BOZEK², INGO FISCHER¹, and REINHOLD FINK³ — ¹University of Würzburg, Germany — ²Synchrotron SOLEIL, Saint-Aubin, France — ³University of Tübingen, Germany

Isothiocyanic acid, HNCS, is the simplest isothiocyanate and a molecule of astrochemical interest. In 1979 it was first detected in the interstellar medium towards the molecular cloud Sgr B2(OH).^[1] The detection of HNCS in space is intriguing due to its composition of biogenic elements. Its oxygen analogue isocyanic acid, HNCO, is a well-known astrochemical molecule for which a prebiotic role was suggested.^[2] Investigating the interaction of HNCS with X-ray radiation is critical to understanding its fate in space.

Here we present the gas phase Auger electron spectra of the reactive molecule isothiocyanic acid that were recorded at the PLEIADES beamline at the synchrotron SOLEIL. X-ray photoelectron and NEX-AFS spectra were obtained and the normal and resonant Auger-Meitner processes were studied at the N1s, C1s and S2p edge. We compare our spectra to the previously recorded spectra of isocyanic acid as well as to theoretical simulations in order to give further insights into the observed transitions and the influence of heavy atom substitution on Auger electron spectra.

[1] M. A. Frerking *et al.*, *Astrophys. J.* **1979**, *234*, L143-L145.

[2] E. Mendoza *et al.*, *Mon. Not. R. Astron. Soc.* **2014**, *445*, 151-161.

MO 20.2 Wed 17:00 Tent

Towards laser spectroscopy of highly excited states of H₃⁺ — ●MARLEEN MAXTON, LUKAS BERGER, FLORIAN GRUSSIE, OLDŘICH NOVOTNÝ, VIVIANE C. SCHMIDT, AIGARS ZNOTINS, and HOLGER KRECKEL — Max-Planck-Institut für Kernphysik, Heidelberg

The H₃⁺ ion is the simplest polyatomic molecule. Apart from being an important benchmark for theoretical calculations, H₃⁺ is one of the main drivers of astrochemistry in dilute interstellar clouds. Despite the structural simplicity of H₃⁺, its spectrum at higher excitation remains largely unexplored, with the highest reported transition occurring at around 16 500 cm⁻¹ with respect to the ground state, less than halfway from the dissociation energy of 35 000 cm⁻¹. To extend the reach of laser spectroscopy beyond previous limits, a concept for a multi-color spectroscopy scheme was proposed [1]. In this approach, highly excited states are populated from the lowest ground states via long-lived metastable intermediates in a two-step laser excitation process, followed by UV photodissociation. For such studies, the Cryogenic Storage Ring (CSR) at the Max-Planck-Institut für Kernphysik provides an ideal platform, combining long storage times for intermediate state population with highly sensitive detection of the dissociation products in an almost background free cryogenic environment. A rotationally cold molecular ion beam is produced by a supersonic expansion source, stored in the CSR and probed for extended periods of time. Currently, the first excitation step is being implemented at the CSR, with plans to realize the full spectroscopy scheme in the future.

[1] Znotins *et al.*, *J. Mol. Spectrosc.* **378**, 111476 (2021)

MO 20.3 Wed 17:00 Tent

A new setup for Free Electron Laser based photoelectron spectroscopy — ●NISHITA LAKHANPAL, KARIMAN ELSHIMI, BERND VON ISSENDORFF, and FABIAN BÄR — University of Freiburg

The development of intense light sources in the XUV and X-ray ranges opens new avenues for the study of free clusters and nanoparticles. A new setup for photoelectron spectroscopy is currently under construction to investigate size-selected, deeply cold clusters, with a focus on characterizing ultrafast electronic processes. This setup will en-

able the exploitation of the vast potential of FELs in photoelectron spectroscopy. Several components, such as the magnetic bottle photoelectron spectrometer, cluster source, and specialized ion optics, are already in place. Additional components, including a QMS, deflector, and ion trap, are still under development.

[1] Bär, F. High-resolution photoelectron spectroscopy on cold metal clusters (Albert-Ludwigs-Universität Freiburg, 2023); <https://doi.org/10.6094/UNIFR/237632>

MO 20.4 Wed 17:00 Tent

Interaction of nitro-compounds with asymmetric ($\omega/2\omega$) fs laser fields — ●PANAGIOTIS VAMVAKIDIS and CONSTANTINE KOSMIDIS — Department of Physics, University of Ioannina, Ioannina 45110, Greece

The focus of our work is to deepen our understanding and, potentially, control the processes of molecular bond rearrangement using asymmetric femtosecond (fs) laser beams. These processes may lead to isomerization and therefore to a change in molecular properties. The studied nitro-compounds have attracted research interest for many years because they are energetic molecules which contribute significantly to "brown carbon" and are also important in biological, pharmaceutical and pesticide applications [1], [2]. Of particular interest is their isomerization processes from nitro (-NO₂) to nitrite (-ONO) structure.

The asymmetric $\omega/2\omega$ fs laser fields are created by spatial and temporal overlapping of the ω ($800 \leq \lambda \leq 2000$ nm) frequency beam with its second harmonic (2ω) ($400 \leq \lambda \leq 1000$ nm) [3]. Interest in this interaction stems from the presence of charge-transfer electronic states within nitro-compounds. By varying the relative phase of the two pulses we can change the shape of the asymmetric field and thus control the distribution of the electronic cloud on the molecular skeleton which offers the ability to (possibly) manipulate their isomerization.

[1] J. M. Shusterman *et al.* *J. Phys. Chem. A*, (2022)

[2] A. D. Tasker *et al.* *J. Phys. Chem. A*, (2002)

[3] E. Kechaoglou *et al.* *J. Chem. Phys.*, (2021)

MO 20.5 Wed 17:00 Tent

Investigating Photoinduced Dynamics of a 1,4-Azaborine with Time-Resolved X-ray Spectroscopy — ●KATHARINA THEIL¹, INGO FISCHER¹, JONAS FACKELMAYER¹, MERLIN HESS¹, HOLGER BRAUNSCHWEIG¹, CONSTANT SCHOUDER², DENNIS MAYER³, FABIANO LEVER³, XIAOJUN WANG³, RUI PAN³, ULRIKE FRÜHLING³, CHRISTINA PAPADOPOULOU³, MARKUS GÜHR³, XINCHENG MIAO¹, SIMONE VEGLIANTI¹, and ROLAND MITRIC¹ — ¹University of Würzburg, Germany — ²ISMO, ParisSaclay University, France — ³DESY, Hamburg, Germany

Azaborines are molecules containing boron and nitrogen, offering unique electronic properties by replacing carbon bonds in organic compounds. This makes them promising for energy and electronic applications, such as optoelectronics and singlet fission materials. In this study, the ultrafast dynamics of the non-commercial 1,4-di-tert-butyl-azaborine were studied using time-resolved X-ray photoelectron spectroscopy. Experiments at FLASH2 at DESY used a pump-probe setup to investigate boron-specific electronic changes after UV excitation. Key processes, including fast relaxation via a conical intersection and slower long-term dynamics, were observed. Supported by static theoretical calculations and quantum dynamic simulations, the study provided insights into excitation energies, long-lived reaction products, and detailed relaxation pathways. These findings highlight the potential of 1,4-azaborines as versatile building blocks for optoelectronic materials, where understanding ultrafast dynamics is key to optimizing performance.

MO 20.6 Wed 17:00 Tent

Detailed investigation of unexpected photoelectron spectra

via angle-resolved spectroscopy of Gold clusters — ●STEVE TAKOUAN TCHOUNGA, LUCAS 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]. In the experiment cluster anions are produced in a magnetron sputter source, cooled to 7K, and enter a time-of-flight spectrometer for mass selection. Electrons are then detached by linear polarised laser light and projected onto an MCP detector in a velocity map imaging setup.

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. It also differs from the mixed character as observed for Sodium clusters of the same size [2]. Possible influences of the high-lying d-band are discussed.

[1] A. Piechaczek, C. Bartels, C. Hock, J.-M. Rost, and B. v. Issendorff, *Phys. Rev. Lett.* (2021), 126.

[2] C. Bartels, C. Hock, R. Kuhnen, M. Walter, and B. v. Issendorff, *Phys. Rev. A* (2013), 88.

MO 20.7 Wed 17:00 Tent

Photoelectron spectroscopy study of cold anthracene anions in gas phase — ●KEVIN SCHWARZ and BERND VON ISSENDORFF — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Organic semiconductors like anthracene ($\text{C}_{14}\text{H}_{10}$) show interesting properties and keep being of interest across science and technology. In modified form they are used, for instance, in organic solar cells. To get a better understanding of these molecules, they are investigated in the gas phase by anion photoelectron spectroscopy (PES), providing insight into the vibrational modes of the electronic ground state and different electronically excited states of the neutral molecule as well as into electronic relaxation processes within the anion. As published previously [1], the photoelectron spectra exhibit strong photon energy-dependent changes in the vibrational excitation of the molecule. These changes result from photoemission via autodetaching excited states of the anion. Seven of eight different identified electronic excitations correspond to resonances of the anthracene anion known from absorption spectroscopy [2]. Recently, a cryogenic radio frequency hexapole ion trap was added to the device, with the goal to study the temperature dependence of the observed ultrafast relaxation processes. New results will be presented.

[1] A. Jalehdoost, B. von Issendorff, *J. Chem. Phys.* 158: 194302 (2023). DOI: <https://doi.org/10.1063/5.0145038>

[2] T. Shida and S. Iwata, *J. Chem. Phys.* 56: 2858-2864 (1972). DOI: <https://doi.org/10.1063/1.1677618>

MO 20.8 Wed 17:00 Tent

Time-resolved Imaging of CH₄ Fragmentation in Strong Laser Fields — ●NIKOLAS RAPP, WEIYU ZHANG, THOMAS PFEIFER, and ROBERT MOSHAMMER — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

With a Reaction Microscope (ReMi) [1] the ionization and dissociation dynamics of methane in strong laser fields were studied in a series of pump-probe experiments. For the creation of temporally separated laser pulses and pulse shaping a spatial light modulator (SLM) was used. It allows the control of laser pulses in terms of amplitude, polarization, and phase [2, 3]. By employing the SLM technique, we successfully compressed the laser pulses to below 10 fs and achieved a precise control over the time-delay between the two pulses. Upon strong-field ionization the molecule undergoes fragmentation and Coulomb explosion (CE) and the corresponding charged fragments are collected with the ReMi. For example, in the case of CE the initial inter-nuclear distances can be determined via the measurement of final kinetic energies, and in pump-probe measurements the evolution of the molecular geometry is visualized as function of time. Selected results will be presented and discussed.

References:

[1] J. Ullrich et al., 2003, *Rep. Prog. Phys.* 66, 1463-1545

[2] Stefanie Kerbstadt, 2016, MA thesis. Universität Oldenburg

[3] T Brixner and G Gerber, 2001, *Opt. Lett.* 26,557-559

MO 20.9 Wed 17:00 Tent

In search for superconductivity in Niobium clusters — ●MAZIYAR KAZMEI and BERND VON ISSENDORFF — Physikalisches Institut Universität Freiburg

Among the superconducting materials, Nb stands out due to its high critical temperature and is often used as a model system, to investigate superconductivity-related physics. The question arises at what size Nb clusters will exhibit properties related to superconductivity, namely Cooper pair formation. Some hints for this to happen already at small sizes have been found by de Heer and coworkers [1]. We have measured photoelectron spectroscopy of size-selected Nb clusters in similar size ranges, with temperatures between 3.9-50 K in the gas phase, employing a recently developed photoelectron magnetic bottle spectrometer with a resolution of $\Delta E/E = 0.2\%$. Vibrationally resolved spectra have been obtained for several sizes, but no direct evidence for unusual temperature effects yet.

MO 20.10 Wed 17:00 Tent

Toward understanding ultrafast dynamics of uracil and uraci-water clusters — ●ADITI PRADHAN^{1,2}, IVO S. VINKLÁREK¹, HUBERTUS BROMBERGER¹, SEBASTIAN TRIPPEL^{1,3}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Chemistry, Universität Hamburg, Germany — ³The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

The solute-solvent interactions in biomolecule-water clusters remain underexplored at ultrafast timescales with atomic scale precision. Studying solvated clusters at the same level of detail as single isolated molecules is a significant challenge. We propose a bottom-up approach to tackle this. The versatile transportable endstation for controlled molecule (eCOMO) [1] employs the electrostatic deflector in combination with velocity map imaging to study clusters in a size-selected fashion [2]. Examining systems with multiple water molecules attached to the building blocks of life, we aim to advance the understanding of ubiquitous interactions like hydrogen bonding. Preliminary experiments on uracil-water clusters reveal interesting dynamics following strong-field ionization. Further UV-photoinduced dynamics of these important model systems will be studied using short-pulse laser sources as well as short-wavelength facilities.

[1] Jin *et al.* (8 authors), Küpper, arXiv:2406.16491 [physics]

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

MO 20.11 Wed 17:00 Tent

Towards Unravelling Solvation Dynamics: From Isolated Molecules to Micro-Hydrated Environments — ●DEEPAK K. PANDEY¹, LILIANA M. RAMOS MORENO¹, CLAUS-PETER SCHULZ², and JOCHEN MIKOSCH¹ — ¹Institut für Physik, Universität Kassel, Kassel, Germany — ²Max Born Institute (MBI), Berlin, Germany

Exploring the behavior of micro-solvated molecules is vital for bridging our understanding of isolated molecules in bulk-liquid environments. Through the gradual addition of water molecules one at a time, our research explores the effects of solvation on neutral molecules. We employ Photoelectron Photoion Coincidence (PEPICO) spectroscopy to investigate both the static and dynamic effects of solvation. Our experimental setup at the University of Kassel employs a water cluster technique to systematically investigate how micro-hydration affects molecular behavior. Using ultrafast pump-probe experiments, this technique enables us to investigate how solvation affects photochemical processes such as photodissociation and photo-induced isomerization. In the past year, we have achieved coincidence measurements with our PEPICO spectrometer, making significant progress in characterizing our water cluster source. With the goal to gain greater insight into the dynamics of micro-hydrated chiral molecules, we intend to include the time-resolved Photoelectron Circular Dichroism (PECD) investigations in the future. Our poster emphasizes on the experimental methodology, analysis of the water cluster source and spectrometer, and progress made in experimental techniques for investigating the molecular dynamics of chemical processes.

MO 20.12 Wed 17:00 Tent

Dynamics of the activation of small molecules by zirconium cations in the gas phase — ●BORIS HEEB, MARCEL META, and JENNIFER MEYER — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

The reaction of Zr^+ with CH_4 in the gas phase proceeds efficiently to the carbene $ZrCH_2^+$ at room temperature with a two-state reactivity along the reaction coordinate [1]. To investigate the bond activation of CH_4 by Zr^+ , energy and angle differential cross sections were recorded by crossed-beam velocity map imaging. The product ion velocity distribution is dominated by signatures of indirect dynamics commonly associated to a small impact parameter. Additional scattering events outside the kinematic limits are found, which largely disappear when switching to CD_4 . A comparison with the reactions $Ta^+ + CH_4$ and $Ta^+ + CD_4$ show almost identical energy and angular distributions [2]. Continuing experiments with 1-butene show three product channels, whereby a mainly forward-scattered distribution is observed for the loss of H_2 , which supports the considerations.

MO 20.13 Wed 17:00 Tent

Photofragmentation studies of cold deoxyadenosine monophosphate (dAMP) anions — ●MIRIAM WESTERMEIER, CHRISTIAN SPRENGER, SAMUEL WHITE, ERIC ENDRES, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

dAMP is a nucleotide which makes up one part of the DNA. It is likely involved in the mutation of genes, if the dAMP is wrongly incorporated into the DNA. Such a mutation could occur when a G to T (guanine to thymine) transversion happens. [1] dAMP consists of a sugar group, a phosphate group and the nucleobase adenine. The phosphate and the sugar form the phosphate-sugar-backbone of a DNA strand. The adenine in this case can form a hydrogen bond with a nucleobase of the second strand. It is possible to fragment the dAMP with ultraviolet light, but the absolute cross-section of this interaction is still unknown. Also the dependence of the fragment branching ratio on the dissociation wavelength is of interest. With our setup, consisting of an electrospray ionization source, an octupole, a quadrupole coupled to a cryogenic 16-pole wire ion-trap and a time-of-flight mass spectrometer, we are studying the absolute cross section of the photofragmentation, and carry out a wavelength scan as well as study the dependence of the fragment yield on the wavelength.

[1] Piette J., Biological consequences associated with DNA oxidation mediated by singlet oxygen. *J. Photochem. Photobiol. B*, 11, 241 (1991)

MO 20.14 Wed 17:00 Tent

Probing De-excitation and Vibrational Re-Distribution Processes in Jet-Cooled N_2O Using a Combination of cw-Infrared and Microwave Chirped Pulse Technique — ●JONAS BOSMANN, FABIAN PETERS, JAN WENSKKE, GUIDO FUCHS, and THOMAS GIESEN — Institute of Physics, University of Kassel, Germany

Chirped pulse Fourier transform spectroscopy (CP-FT) is a sensitive and nowadays widely used method for recording gas phase spectra of molecules in the microwave (MW) and millimeter wave (mmW) range. Here, we present CP-FT supersonic beam measurements of N_2O , state selectively excited by an infrared continuous wave (cw) optical parametric oscillator (OPO). The CP-FT signal of the $J = 4 \leftarrow 3$ transition around 100 GHz was used to study the relaxation of vibrationally excited N_2O into different vibrational levels of lower energy. Since this is to our knowledge the first CP-MW study that uses cw-laser excitation, we investigated the strength of the FID signal as a function of the infrared laser power. The collision-induced redistribution of pure rotational levels in vibrationally states and the redistribution of vibrational energy were investigated in two different jet environments, for which a slit nozzle of high collision rates and a pin-hole nozzle of low collision rates in the jet expansion were used.

MO 20.15 Wed 17:00 Tent

3D Time Resolved Photoelectron Spectroscopy on Carbondisulfide — ●MARVIN KRUPP¹, SCOTT GOUDREAU², ANDREY BOGUSLAVSKIY², JEAN-LUC BÉGIN², and ALBERT STOLOW² — ¹Institute of Physics, University of Rostock, 18059 Rostock, Germany — ²Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada

Time-resolved photoelectron spectroscopy (TRPES) is a versatile probe of ultrafast dynamics in molecules and has been widely used in recent years to study non-adiabatic dynamics in numerous systems. Here, the 2D photoelectron velocity map imaging (VMI) technique is commonly employed in gas-phase molecular spectroscopy and dynamics investigations due to its ability to efficiently extract photoelectron spectra and angular distributions in a single experiment. However, the standard technique is limited to specific light-source polarization

geometries. This has led to significant interest in the development of 3D VMI techniques, which are capable of measuring individual electron positions and arrival times, obtaining the full 3D distribution without the need for inversion, forward-convolution, or tomographic reconstruction approaches. Time resolved photoelectron spectra of the $^1B_2(^1\Sigma_u^+)$ -state of CS_2 at pump wavelengths in the region of 200 nm have been previously studied and indicate that the lifetime of the decay is dependent on the relative laser polarisation geometry. In this work, we present the first results employing the new 3D VMI technique on CS_2 and comparing it with the previous 2D VMI study.

MO 20.16 Wed 17:00 Tent

Imaging thermal-energy chemical dynamics of a solvated (bio)molecular complex system — ●MUKHTAR SINGH^{1,2,3}, MATTHEW SCOTT ROBINSON^{1,2,3}, HUBERTUS BROMBERGER^{1,2}, SEBASTIAN TRIPPEL^{1,2}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Center for Ultrafast Imaging, Universität Hamburg — ³Department of Physics, Universität Hamburg

We present the imaging of ultrafast thermal-energy-induced chemical dynamics of a micro-solvated indole-water molecular complex probed with a time-dependent strong field ionization and ion mass spectrometry [1]. We produce a pure gas-phase indole-water sample using a combination of a cold molecular beam and the electrostatic deflector [2]. Employing a 2.9 μm mid-IR pump to excite the N-H and C-H vibrational modes induced dynamics between the indole and water moieties.[3]. The dissociation of the micro-solvated system was monitored using strong-field multi-photon ionization by 1.3 μm wavelength light from a femtosecond pulsed laser, tracking the time-dependent ion signals of the intact indole-water cluster as well as the individual indole and water ionic products.

[1] J. Onvlee, *et al.*, *Nat. Commun.* **13**, 7462 (2022).

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

[3] M.S. Robinson, *et al.*, *Phys. Chem. Chem. Phys.* (2023).

MO 20.17 Wed 17:00 Tent

UV photo-induced dissociation dynamics of solvated (bio)molecular complex system — ●MUKHTAR SINGH^{1,2,3}, MATTHEW SCOTT ROBINSON^{1,2,3}, HUBERTUS BROMBERGER^{1,2}, SEBASTIAN TRIPPEL^{1,2}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Center for Ultrafast Imaging, Universität Hamburg — ³Department of Physics, Universität Hamburg

We present the investigation of ultrafast chemical dynamics induced by UV excitation in a micro-solvated indole-water-complex system probed by time-dependent strong-field ionization and ion mass spectroscopy [1]. Indole-water is important due to indole's role as the chromophore of tryptophan, the strongest near UV absorber in proteins. The experimental setup contains a molecular beam and the electrostatic deflector to produce a pure gas-phase sample of indole-water [2]. We conducted a UV-IR pump-probe experiment, which excited the system to the electronic excited state using 270 nm light. The dissociation dynamics of the system was monitored using strong-field multiphoton ionization by 1.3 μm wavelength light from a femtosecond laser, tracking the time-dependent ion signals of the indole and indole-water ions and electrons.

[1] J. Onvlee, *et al.*, *Nat. Commun.* **13**, 7462 (2022).

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

MO 20.18 Wed 17:00 Tent

Simplifying rotational spectra: A broadband double resonance approach in millimeter wave spectroscopy — ●PRACHI MISRA, LUIS BONAH, MARIYAM FATIMA, and STEPHAN SCHLEMMER — I. Physikalisches Institut, Universität zu Köln, Köln, Germany

Rotational spectroscopy is an important technique for understanding molecular structures, as rotational constants are directly linked to the molecular mass distribution and interatomic distances. In Cologne, high-resolution rotational spectra are measured using Chirped-Pulse Fourier Transform (CP-FT) spectroscopy¹ in gas phase.

Analyzing rotational spectra for complex molecules is often complicated by weak features arising from low-lying vibrationally excited states, hyperfine splitting, and internal rotation. To address these challenges, the well-established technique double-resonance spectroscopy is employed. This method uses a probe radiation source to record spectra while a pump source modifies specific transitions due to the Autler-Townes effect. By identifying the connected transitions we can piece together the energy term diagram experimentally. This technique has

previously been implemented using absorption spectroscopy², and is now adapted for use with CP-FT spectroscopy allowing for broadband coverage, eliminating the need for frequency-by-frequency scanning of both the pump and probe radiation sources. Proof-of-concept experiments conducted in the 75-110 GHz range using a new signal generation and acquisition board on the CP-FT spectrometer³ are presented.

1. Park, G.B. (2016) *J. Chem. Phys.*, 144(20) 2. Zingsheim, O. (2021) *J. Mol. Spectrosc.*, 381, 111519 3. Hermanns, M., (2023) *Rev. Sci. Instr.*, 94(3)

MO 20.19 Wed 17:00 Tent

Investigation of the interaction between organic dopants and a helium nanodroplet environment with time-resolved photoelectron spectroscopy — ●LEONIE WERNER, ULRICH BANGERT, SEBASTIAN HARTWEG, YILIN LI, ARNE MORLOK, FELIX RIEDEL, FRANK STIENKEMEIER, and LUKAS BRUDER — University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg im Breisgau, Germany

Embedding molecules in ultracold helium nanodroplets allows us to study molecular processes in a superfluid environment [1]. Here, we apply time-resolved photoelectron spectroscopy to study the dynamics of dopants embedded in helium nanodroplets. Droplet size-dependent photoelectron spectra [2] have been established as an appropriate technique for studying interactions between organic dopants and the helium environment. Probing helium droplets doped with selected organic molecules, we present a systematic study of the evaporation and ejection dynamics upon laser excitation. Both phenomena have been observed previously in helium nanodroplets for different dopants [1,3,4]. First results will be presented, in particular on ultrafast internal conversion in tetracene.

[1] Toennies, J.P. and Vilesov, A. F. (2004), *Angew. Chem.*

In. Ed. 43(20): 2622-2648

[2] Loginov, E. et al. (2005), *Phys. Rev. Lett.* 95(16): 163401

[3] Thaler, B. et al. (2018), *Nat. Commun.* 9(1): 4006

[4] Meyer, M. et al. (2019), *EPJ Web Conf.* 205: 06005

MO 20.20 Wed 17:00 Tent

Photodissociation dynamics of the bromomethyl radical — ●LILITH WOHLFART, CHRISTIAN MATTHAEI, and INGO FISCHER — JMU Würzburg, Germany

Bromomethyl belongs to the class of organic halogen radicals. Therefore, it can potentially influence the atmosphere by reacting with the ozone layer and causing its depletion similar to HCFCs. The photoionization of bromomethyl was already investigated by several groups, including Steinbauer and coworkers. They determined the ionization energy and structure with VUV synchrotron radiation and investigated the dissociative photoionization. To obtain further insights into the dissociation of bromomethyl, we analyzed the fragments of the radical using velocity map imaging (VMI).

CH₂Br-NO₂ was used as a precursor for the halogenated methyl radical, because the weaker C-NO₂ bond can be cleaved through pyrolysis. Subsequently, laser light in the UV region was deployed to dissociate the formed CH₂Br radical. The major dissociation pathway gave the methylene and bromine fragments which were detected with SPI and REMPI respectively. With velocity map ion imaging, the translational kinetic energy distribution of the photofragments was determined. The

recorded images of the bromine and methylene photofragments showed an anisotropic distribution, implying a direct dissociation.

MO 20.21 Wed 17:00 Tent

Generation of long-lived triplet-triplet multiexciton in Pentacene-(Tetracene)2-Pentacene intramolecular singlet fission compound - the theoretical perspective. — ●ARIFA NAZIR¹, ALOK SHUKLA², and SUMIT MAZUMDAR³ — ¹Indian Institute of Technology Bombay — ²Indian Institute of Technology Bombay — ³University of Arizona

Singlet fission (SF) is a spin-allowed conversion of the optical singlet exciton of an organic semiconductor to the optically dark triplet-triplet (¹(T₁T₁)). In chromophores with small triplet-triplet binding energy ¹(T₁T₁) can separate into two free triplets T₁, each of which can donate an electron to an acceptor, thereby doubling the photoconductivity of an organic solar cell. Successful implementation of SF requires both ultrafast generation of the ¹(T₁T₁) and rapid dissociation into free triplets, which is a challenge, as the former requires strong coupling between the triplets, which implies strong ¹(T₁T₁) binding energy. Pun et al. synthesized a series of oligomers Pentacene-(Tetracene)_n-Pentacene, P_nT_nP, in which rapid generation of pentacene-tetracene triplet-triplet ¹(T₁[P]T₁[T]) is followed by rapid triplet separation to long-lived pentacene-pentacene triplet-triplet ¹(T₁[P]T₁[P]) [1]. We present the results of many-body investigations of the electronic structures of the optical singlet and low-energy triplet-triplets in PT2P that find distinct ¹(T₁[P]T₁[T]) and ¹(T₁[P]T₁[P]). We also report the ground and excited state absorptions that clarify triplet-triplet generation and triplet separation mechanisms. [1] A. B. Pun et al., *Nat. Chem.* 11, 821 (2019).

MO 20.22 Wed 17:00 Tent

Coulomb explosion imaging of molecular photoswitches — KIERAN CHEUNG¹, ARNAUD ROUZEE², CLAUS PETER SCHULZ², TILL JAHNKE³, DAVID BUSTO⁴, PER ENG-JOHNSSON⁵, REBECCA BOLL⁶, MARC J. J. VRAKING¹, GIUSEPPE SANSONE⁴, DANIEL ROLLES⁷, MICHAEL MEYER⁶, TERRY MULLINS⁶, MARK BROUARD¹, and ●KASRA AMINI² — ¹Chemistry Research Laboratory, Department of Chemistry, University of Oxford, Oxford OX1 3TA, UK — ²Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin, Germany — ³Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — ⁴Physikalisches Institut, Universität Freiburg, 799104 Freiburg, Germany — ⁵Department of Physics, Lund University, Lund, Sweden — ⁶European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany — ⁷J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Kansas 66506, USA

We present an X-ray Coulomb explosion imaging (CEI) investigation into the photofragmentation and photochemistry of trans-4,4'-difluoroazobenzene (DFAB) using the COLTRIMS Reaction Microscope at the SQS station of the European XFEL. We show a systematic analysis of X-ray-induced fragmentation in DFAB, employing covariance techniques to explore fragmentation dynamics. We then report time-resolved measurements of DFAB excited to its first electronic excited state (*S*₁) under varying visible pump excitation conditions. Our findings highlight the limited propensity of trans-DFAB to undergo trans-to-cis isomerization following *S*₁ excitation and reveal the emergence of a dissociative ionization process leading to photodissociation.

MO 21: Poster – Interaction with Strong or Short Laser Pulses (joint session A/MO)

Time: Wednesday 17:00–19:00

Location: Tent

MO 21.1 Wed 17:00 Tent

Towards Multidimensional XUV Spectroscopy Combined with Spectral Interferometry — ●LINA HEDEWIG^{1,2}, CARLO KLEINE¹, FELIX WIEDER^{1,2}, CHRISTIAN OTT^{1,2}, and THOMAS PFEIFER^{1,2} — ¹Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — ²Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg, Germany

Using up to two infrared (IR) and two extreme ultraviolet (XUV) ultrashort pulses we are currently implementing a method for multidimensional XUV spectroscopy combined with spectral interferometry to gain further insight into gas-phase quantum dynamics of atoms and molecules.

The setup is based on a four-quadrant split-and-delay mirror al-

lowing independent time delay control of each beam. In situ phase correction results in an effective interferometer stability of 1.5 attoseconds. One XUV pulse excites an electronic wave-packet in the target generating a coherent dipole response. This wave-packet is strongly coupled by the two IR pulses, leading to control of state-specific quantum dynamics as well as the signal's diffraction towards the remaining fourth beam for a nearly background-free detection. To additionally extract the dipole response's phase, the second XUV beam serves as local oscillator for heterodyned spectral interferometry. The additional phase information compared to classical transient absorption opens up a plethora of possibilities like pulse reconstruction beyond the single-atom response, improved robustness against detector intensity noise and dipole reconstruction for short dipole lifetimes.

MO 21.2 Wed 17:00 Tent

Universal Behavior of Tunneling Time and Disentangling Tunneling Time and Barrier Time-Delay in Attoclock Experiments — ●OSSAMA KULLIE¹ and IGOR IVANOV² — ¹Theoretical Physics, Department of Mathematics and Natural Science, University of Kassel, Germany — ²Department of Fundamental and Theoretical Physics, Australian National University, Australia

In a model we showed that the (tunnel-ionization) time-delay measured by the attoclock experiment can be described accurately in adiabatic and nonadiabatic field calibrations. Moreover, the barrier tunneling time-delay itself can be determined from the difference between the time-delay of adiabatic and nonadiabatic tunnel-ionization, showing good agreement with experimental results. What is particularly striking and interesting is that we have shown that the tunneling time exhibits a universal behavior with disentangled contributions. In Addition, we find that the weak measurement limit, the barrier time-delay corresponds to the Larmor-clock time and the interaction time within the barrier. [1] Submitted to J. Phys. Comm. (2024). [2] Kullie and I. Ivanov, *Annals of Physics* 464, 169648 (2024). [3] Kullie, *Phys. Rev. A* 92, 052118 (2015).

MO 21.3 Wed 17:00 Tent

Towards Imaging Electron Dynamics in Solids with Attosecond Resolution — ●MATTHIAS MEIER¹, MARTIN REH¹, YUYA MORIMOTO², FRANCESCO TANI³, and PETER HOMMELHOFF^{1,3,4} — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — ²RIKEN Cluster for Pioneering Research (CPR) and RIKEN Center for Advanced Photonics (RAP), Japan — ³Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — ⁴Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

The understanding and precise control of electron dynamics in solids plays a key role for the development of new technologies. However, investigating the time-resolved dynamics on the timescale of femto- to attoseconds proves to be a persistent challenge. One way to overcome this issue is by optically probing the dynamics on the very same timescale. For this aim, isolated attosecond pulses (IAP) present a sharp and distinct measurement tool which is ideally suited to investigate these ultrafast mechanisms. Here, we present the pulse compression of 20 μJ pulses at a central wavelength of 1030 nm and a width of 225 fs down to few cycle pulses which are used to generate XUV light by driving a high-harmonic generation process. Adjusting the stabilized carrier-envelope phase together with a short-pass filter allows to generate IAP. Combining the IAP with a copy of the driving field in an ultrashort pump-probe scheme enables the observation of electron dynamics in the attosecond time scale.

MO 21.4 Wed 17:00 Tent

Strong-Field Ionization and Laser-Driven Electron Recollision of Molecules studied in a Reaction Microscope — ●NARAYAN KUNDU¹, MARTIN GARRO¹, JANKO JANKO UMBACH¹, HORST ROTTKE¹, TOBIAS WITTING², ARNE SENFTLEBEN¹, and JOCHEN MIKOSCH¹ — ¹Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ²Ultrafast XUV-Physics, Max Born Institute (MBI), Max-Born-Straße 2A, 12489 Berlin, Germany

Reaction microscopes (REMI) are among the most powerful spectrometers in experimental AMO physics. In a REMI, the momentum of multiple electrons and ions resulting from an event can be measured in coincidence. Here we present experiments on isolated molecules, which are ionized with an intense, femtosecond laser field. In current work on Strong-Field Ionization of 1,3-butadiene, n-butane, and 1-butene molecules, we varied intensities and wavelengths. We observe qualitative changes of experimental observables as a function of these parameters, which we interpret as transition between non-sequential and sequential excitation processes in the intense field. We also present our progress towards using Strong-Field Ionization as a probe mechanism for molecular dynamics and on laser-driven elastic rescattering in a chiral molecule. Furthermore, we have set up a post-compression scheme to significantly reduce the pulse duration of the laser pulses from our commercial regenerative amplifier, based on a gas-filled hollow-core fiber with pressure gradient and chirped mirrors.

MO 21.5 Wed 17:00 Tent

Electron-nuclear dynamics in dissociative strong-field ionization of D₂ — ●PAUL WINTER and MANFRED LEIN — Leibniz University Hannover, Germany

In a neutral diatomic molecule, the removal of an electron by a strong field is a much faster process than the subsequent breakup of the ionized molecule, primarily due to the significant difference in mass between the rapidly moving electrons and the considerably heavier nuclei. This mass disparity also suggests that during strong-field ionization with a linearly polarized pulse, the rescattering electron may not significantly affect molecular dynamics. If, however, electrons rescatter inelastically with the core, vibrational excitation could take place [1].

To explore this mechanism, we have developed a non-Born-Oppenheimer model in which we solve the time-dependent Schrödinger equation (TDSE), treating the electron in two dimensions and the internuclear motion in one dimension. Additionally, we have incorporated the first excited state of the ionized molecule to account for typical dissociation phenomena such as bond-softening and above-threshold dissociation (ATD). With this model, we can calculate photoelectron momentum distributions (PMDs) as a function of the kinetic energy release of the nuclei, paving the way for detailed studies of coupled electron-nuclear dynamics.

[1] S. Hell, G.G. Paulus, M. Kübel, private communication

MO 21.6 Wed 17:00 Tent

Modeling controlled sub-wavelength plasma formation in dielectrics — ●JULIA APPORTIN, CHRISTIAN PELTZ, BJÖRN KRUSE, BENJAMIN LIEWEHR, and THOMAS FENNEL — Institute for Physics, Rostock, 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 modelling aiming at improving user control over these modifications. In particular the associated feedback effects on the field propagation can have drastic implications.

We developed and utilized a numerical model, that combines a local description of the plasma dynamics in terms of corresponding rate equations for ionization, collisions and heating 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. Here we present recent numerical results regarding the creation and control of sub-wavelength gratings formed at the rear side of pure and gold-coated fused silica films.

[1] L. Englert et al, *Opt. Express* 15, 17855-17862 (2007)[2] M. Alameer et al, *Opt. Lett.* 43, 5757-5760 (2018)

MO 21.7 Wed 17:00 Tent

Cross-process interference in single-cycle electron emission from nanotips — ●ANNE HERZIG, THOMAS FENNEL, and LENNART SEIFFERT — Institute of Physics, University of Rostock, 18059 Rostock, Germany

Photoelectron spectra from strong-field ionization show features like energy cutoffs and interference patterns, influenced by direct and backscattered electrons [1]. The typical cut-offs at $2U_p$ and $10U_p$ can be explained within the famous three-step model, while quantum inter- and intracycle interferences are typically associated with self-interference of direct or backscattered, respectively [2,3]. However, also cross-process interference (CPI) between direct and backscattered electrons could reveal further insights. To isolate CPI, competing effects from self-interference must be suppressed, achievable with single-cycle laser pulses [4] that confine electron emission to a single optical period. Metallic nanotips further enhance this by restricting electron motion to one half-space, ensuring strong backscattering [5]. Quantum simulations predict CEP-dependent photoelectron spectra with distinct interference patterns. An extended trajectory model confirms these features originate from CPI, offering insights into the underlying physical mechanisms.

[1] F. Krausz et al., *Reviews of Modern Physics* 81, 163-234 (2009)[2] F. Lindner et al., *Physical Review Letters* 95, 040401 (2005)[3] D.G. Arbó et al., *Physical Review A* 74, 063407 (2006)[4] M.T. Hassan et al., *Nature* 530, 66-70 (2016)[5] S. Zherebtsov et al., *Nature Physics* 7, 656-662 (2011)

MO 21.8 Wed 17:00 Tent

Pulsed standing waves at 100 MHz repetition rate for multiphoton ionization experiments — ●JAN-HENDRIK OELMANN, TO-

BIAS HELDT, LENNART GUTH, LUKAS MATT, THOMAS PFEIFER, and JOSÉ R. CRESPO LÓPEZ-URRUTIA — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

We investigate multiphoton ionization (MPI) at high laser intensity (10^{13} W/cm²) and high repetition rate (100 MHz) using a novel polarization-insensitive enhancement cavity for amplified near infrared frequency comb laser pulses. A velocity-map imaging (VMI) spectrometer is integrated into the cavity and allows measuring photoelectron angular distributions (PADs) [1]. By turning the laser polarization axis, we were able to tomographically reconstruct 3D PADs from xenon MPI, revealing resonant Rydberg states during ionization [2].

Additionally, the bow-tie cavity supports counter-propagating pulses forming an intense standing wave at the cavity focus. We use the intrinsic nanometric structure of this standing light field to study and control photoemission from a sharp tungsten tip at the nanometer scale [3]. For gas-phase ionization studies, colliding pulses offer the advantage of reducing the interaction volume at the focus and doubling the intensity [4].

[1] J. Nauta *et al.*, *Opt. Lett.* **45**, 2156 (2020). [2] J.-H. Oelmann *et al.*, *Rev. Sci. Instrum.*, **93**(12), 123303 (2022). [3] T. Heldt *et al.*, *Nanophotonics*, 2024. [4] T. Heldt *et al.*, *Opt. Lett.* **49**, 6825-6828 (2024)

MO 21.9 Wed 17:00 Tent

High-Harmonics Spectroscopy of Vibrating Chains — ●GABRIEL CACERES-ARAVENA and DIETER BAUER — Institute of Physics, University of Rostock, 18051 Rostock, Germany

In this work, we study the High-Harmonic Generation (HHG) of the laser-driven Su-Schrieffer-Heeger (SSH) chain where the electrons are coupled to the local phonons. The electron dynamics is implemented using the tight-binding approximation and the electron-phonon interaction is implemented through the Holstein model, where the local

vibrations of ions are approximated to be solutions of the quantum harmonic oscillator. In our simulations we observe that the electrons move accelerated by the electric field from the driving laser, as expected, and also we observe that the phonons move following the electron movement, showing the existence of a polaron. Also, when we introduce phonons to the system, we observe from the eigenenergy spectrum that new states emerge. Transitions to these new states allow for more efficient harmonic generation for certain harmonic orders.

MO 21.10 Wed 17:00 Tent

Probing electron dynamics in gases and pulse characterization using an interferometric Velocity Map Imaging setup — ●PRANAV SREEKUMAR¹, DAVID SCHMITT¹, SVEN FRÖHLICH¹, UWE MORGNER¹, MILUTIN KOVACEV¹, and ANDREA TRABATTONI^{1,2} — ¹Institut für Quantenoptik, Leibniz Universität Hannover, Germany — ²Center for Free-Electron Laser Science CFEL, DESY Hamburg

The strong-field ionization of rare gases using intense fs laser pulses results in characteristic spectra for photoelectrons in the momentum and energy space. It has been shown that such signatures contain holographic information which can be obtained experimentally with high spatial resolution using a Velocity Map Imaging (VMI) spectrometer for photoelectrons. However, the interpretation of these velocity maps is not straightforward as they often contain signatures arising from multiple phenomena and the isolation of individual signatures is a significant challenge.

In this poster, we will present our setup of an interferometric beamline coupled into a VMI. With our setup, we aim to extract the sub-optical cycle photoelectron holographic signatures, which promises to offer information on electron dynamics within atoms occurring at sub-to-few fs timescales. Besides this, we also demonstrate the capability to perform in-situ pulse characterization, utilizing the higher-order non-linearity associated with strong-field ionization [1].

[1] Geffert *et al.*, *Optics Letters* **47**.16, 3992-3995 (2022)

MO 22: Ultrafast Dynamics III

Time: Thursday 11:00–13:00

Location: HS XVI

MO 22.1 Thu 11:00 HS XVI

Ultrafast Relaxation Dynamics of the Q-Bands in Chlorophyll a in Ethanol — ●LENA BAUML, FERDINAND POINTNER, SEBASTIAN REITER, and REGINA DE VIVIE-RIEDLE — Department of Chemistry, LMU Munich, Germany

The natural pigment chlorophyll adopts different functions during the conversion of sunlight to chemical energy. Depending on its environment, its role in photosynthetic light-harvesting varies significantly.

In this work we investigate the excited states dynamics of chlorophyll *a* in ethanol. In a previously published study^[1], conducted in the gas phase, we focused on the relaxation process after excitation into the *Q*-band. There, we found the *Q_x* and *Q_y* band to be strongly coupled via internal vibrations. It is known, that solvents significantly alter the spectral shape of e.g. absorption or fluorescence spectra and influence the population decay times in the ultrafast relaxation process. Therefore, now the influence of solvent environment, specifically ethanol, on the coupling situation and the relaxation dynamics is under investigation. We present a variation of a QD/MD scheme developed in our group^[2] and discuss the observed changes compared with our results for chlorophyll *a* in the gas phase.

[1] L. Bäuml *et al.*, *Phys. Chem. Chem. Phys.* **24**, 27212 (2022).

[2] S. Reiter *et al.*, *J. Am. Chem. Soc.* **140**, 8714 (2018).

MO 22.2 Thu 11:15 HS XVI

Linear and Two-Dimensional IR Spectroscopy of an Isotopically Labeled Multifunctional Vibrational Probe — ●CLAUDIA GRÄVE, JÖRG LINDNER, STEFAN FLESCHE, LUIS IGNACIO DOMENIANNI, and PETER VÖHRINGER — Clausius-Institute, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Vibrational spectroscopy of biomacromolecules often relies on the introduction of infrared probes, whose vibrations are highly sensitive to the local environment. Here, we report on the prospective IR probe, 3-(4-azidophenyl)propionitrile, which contains several IR-active functional groups.

Its linear FTIR spectrum is highly perturbed in the spectral region

of the asymmetric azide stretching fundamental due to the presence of Fermi resonances. We managed to assign the fundamental transition via isotope labeling of the azide group. In combination with DFT calculations, this allowed us to construct a two-tiered Fermi resonance Hamiltonian to identify the involved combination tones.

Additionally, we performed ultrafast vibrational spectroscopy on the isotopically labeled IR probe. 2D-IR spectra exhibit a delayed appearance of cross-peaks between the azide asymmetric and the in-phase propionitrile stretching modes. Along with narrowband IR-pump/IR-probe spectroscopy, these results reveal an irreversible intramolecular vibrational energy redistribution (IVR) that involves couplings of the two oscillators to different subsets of low-frequency modes. Our data shows a time constant of 2.3 ps for the IVR, whereas energy dissipation to the solvent occurs on a time scale of 18 ps.

MO 22.3 Thu 11:30 HS XVI

Isolating (multi-)exciton dynamics via fluorescence-detected pump-probe spectroscopy — ●STEFAN MUELLER¹, AJAY JAYACHANDRAN¹, CHRISTOPH LAMBERT², and TOBIAS BRIXNER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Action-detected nonlinear spectroscopy has received increasing attention in the past years. While useful, it has recently been identified that action-based nonlinear spectra can be subject to undesired background stemming from incoherent mixing. This effect obscures single-exciton dynamics and is especially dramatic in systems with an increasing number of chromophores [1]. Moreover, inevitable pulse overlap causes artificial multiple-quantum coherences [2]. Both incoherent mixing and artificial multiple-quantum coherence reduce the meaningfulness of action-based spectra and exacerbate their interpretation. Here we introduce a technique that eliminates both undesired contributions. We demonstrate our approach using fluorescence-detected pump-probe spectroscopy (F-PP) on squaraine dimers and polymers. We extract fourth- and sixth-order F-PP spectra to isolate single- and bi-exciton dynamics, respectively, without spurious background. This

works even in polymers which suffer to a particularly large degree from incoherent mixing due to the large number of involved chromophores.

- [1] L. Bolzonello et al., *J. Phys. Chem. Lett.* **14**, 11438 (2023).
 [2] U. Bangert et al., *Opt. Lett.* **48**, 538–541 (2023).

MO 22.4 Thu 11:45 HS XVI

Higher-order signal separation in nonlinear spectroscopy: An intensity-based general approach — ●LUISA BRENNEIS¹, JACOB J. KRICH^{2,3}, PETER A. ROSE², KATJA MAYERSHOFER¹, SIMON BÜTTNER¹, JULIAN LÜTTIG⁴, PAVEL MALÝ⁵, and TOBIAS BRIXNER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Department of Physics, University of Ottawa, Ottawa, ON, Canada — ³Nexus for Quantum Technologies, University of Ottawa, Ottawa, ON, Canada — ⁴Department of Physics, University of Michigan, Ann Arbor, MI, USA — ⁵Faculty of Mathematics and Physics, Charles University, 121 16 Prague, Czech Republic

Nonlinear spectroscopic techniques, like two-dimensional electronic spectroscopy (2DES), are powerful tools for investigating multiparticle correlations and complex dynamics. However, depending on the pulse intensities, the detected signal consists of multiple perturbative orders exhibiting different lineshapes and dynamics. Separating these orders remains a universal challenge, especially while maintaining a high signal-to-noise ratio. Recently, we published an intensity-cycling scheme to extract nonlinear orders in transient absorption spectroscopy [1]. Now we present a generalized version to separate the perturbative orders in a wide range of spectroscopy techniques. In an experimental demonstration, we perform order separation in 2DES of squaraine polymers. We also derive the optimal intensities to minimize the combined effect of random and systematic errors.

- [1] P. Malý et al., *Nature* **616**, 280 (2023).

MO 22.5 Thu 12:00 HS XVI

Resolving higher-order signals through intensity cycling in two-dimensional electronic spectroscopy on the example of a squaraine dimer — ●KATJA MAYERSHOFER¹, JACOB J. KRICH^{2,3}, LUISA BRENNEIS¹, SIMON BÜTTNER¹, PETER A. ROSE², JULIAN LÜTTIG⁴, PAVEL MALÝ⁵, and TOBIAS BRIXNER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Department of Physics, University of Ottawa, Ottawa, Ontario, Canada — ³Nexus for Quantum Technologies, University of Ottawa, Ottawa, Ontario, Canada — ⁴Department of Physics, University of Michigan, Ann Arbor, MI, USA — ⁵Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Recently, we developed a variant of transient absorption spectroscopy that separates different perturbative orders of nonlinear response through “intensity cycling” [1]. We now extend this method, enabling separation of third- and higher-order contributions in two-dimensional (2D) spectra, by multiplication of a Vandermonde matrix with fluence-dependent 2D data. We apply this new method on a squaraine dimer to resolve nonlinear orders, allowing us to analyze uncontaminated signals and compare the lineshapes of different orders of nonlinear response. We perform simulations using the Ultrafast Spectroscopy Suite toolbox [2,3] to gain insight into the differences in lineshapes.

- [1] P. Malý et al., *Nature* **2023**, 616, 280.
 [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 22.6 Thu 12:15 HS XVI

Investigation of Multi-Exciton Interactions in a Chiral Squaraine Homopolymer Employing Higher-Order Pump–Probe Spectroscopy and Fluorescence-Detected Two-Dimensional Spectroscopy — ●KARINA HEILMEIER¹, STEFAN MUELLER¹, EMELY FREYTAG², PETER A. ROSE³, JACOB J. KRICH^{3,4}, CHRISTOPH LAMBERT², and TOBIAS BRIXNER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Ger-

many — ³Department of Physics, University of Ottawa, Ottawa, Ontario, Canada — ⁴Nexus for Quantum Technologies, University of Ottawa, Ottawa, Ontario, Canada

Third-order spectroscopy such as transient absorption (TA) is often used to investigate the dynamics of single-exciton states. The measurement of higher orders provides information on the interactions of an increasing number of excitons and their dynamics. We recently showed how nonlinear orders can be separated using intensity cycling [1]. Here, we study multi-exciton interaction in a related but structurally different chemical system, a chiral squaraine homopolymer. We use intensity-dependent TA to separate odd orders of nonlinear response. In addition, we employ fluorescence-detected two-dimensional spectroscopy. In that case, we extract the even orders by phase cycling and compare the two approaches.

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

MO 22.7 Thu 12:30 HS XVI

Femtosecond-spectroscopy of novel Fe(III)-complexes demonstrating a reservoir effect — ●SAMIRA DABELSTEIN¹, LENNART SCHMITZ², FRANZISKA FENNEL¹, MIGUEL ANDRE ARGÜELLO CORDERO¹, JAKOB STEUBE², MATTHIAS BAUER², and STEFAN LOCHBRUNNER¹ — ¹University of Rostock, Germany — ²Paderborn University, Germany

Conventional photosensitizers for photocatalysis are typically derived from rare and valuable precious metals, prompting the search for alternatives based on first-row transition metals. Among these, iron-based photosensitizers emerge as potential candidates but are limited by their short-lived charge transfer states. To overcome this limitation, targeted ligand design is employed as a strategy. This study presents a series of emitting iron(III) complexes modified with chromophores, featuring either phenyl or anthracene groups. The chromophores are attached to the ligand via a methyl spacer. While the phenyl-extended complexes exhibit behavior similar to the original complex, the anthracene-extended complexes reveal a reservoir effect, characterized by a population transfer from the ligand-to-metal charge transfer state to the triplet state of anthracene. Additionally, a correlation is observed between the number of attached anthracene units and the rate of population transfer. Our findings, obtained through time-resolved methods, specifically femtosecond transient absorption UV-Vis spectroscopy and streak camera measurements, are discussed in detail.

MO 22.8 Thu 12:45 HS XVI

Halide Modulated Excited States of Dinuclear Copper Complexes — ●DANIEL MARHÖFER¹, CLARA ADAM², ANNA MAURI³, MARTIN NIEGER⁴, OLAF FUHR⁵, PATRICK WEIS⁶, GEREON NIEDNER-SCHATTEBURG¹, WOLFGANG WENZEL³, and STEFAN BRÄSE² — ¹Department of Chemistry and State Research Center OPTIMAS, RPTU Kaiserslautern — ²Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT) — ³Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT) — ⁴Department of Chemistry, University of Helsinki — ⁵Karlsruhe Nano-Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT) — ⁶Institute of Biological and Chemical Systems, Functional Molecular Systems (IBCS-FMS), Karlsruhe Institute of Technology (KIT)

Organic Light-Emitting-Diodes (OLEDs) are a key technology in state-of-the-art display applications, offering unparalleled efficiency and color purity. Copper as an earth-abundant metal shows promising characteristics regarding luminescence lifetimes and quantum yields. However, energy efficiency necessitates quantum yields close to 100 % as e.g. achievable through Thermally Activated Delayed Fluorescence (TADF). We investigated by luminescence, time-correlated single photon counting and step-scan FTIR spectroscopy a series of five isostructural, dinuclear copper complexes. Variation of the two (pseudo-)halide ligands modulates excited state lifetimes and luminescence patterns. Our interpretation of the TADF behaviour revealed significant variations of the singlet-triplet gap, beyond obvious trends. Quantum chemical modelling partly challenges these findings.

MO 23: Cluster and Nanoparticles I (joint session MO/A)

Time: Thursday 11:00–13:15

Location: HS XV

Invited Talk

MO 23.1 Thu 11:00 HS XV

Pickup and reactions of molecules on clusters relevant for atmospheric processes — ●JOZEF LENGYEL — Technical University of Munich, Garching, Germany

The uptake of molecules by preexisting clusters in molecular beams is demonstrated using two distinct experiments. In the first one, the doping of hydrated acid clusters with various molecules is investigated. Sticking efficiencies, including uptake cross sections, are determined using the combination of cluster mass spectrometry and velocity measurements. The combined experimental and computational approach provides insights into molecule-cluster collision dynamics, illustrated by a series of measurements involving diverse molecular interactions and steric effects. The second one focuses on the dissociation of nitric acid on large water clusters. While dissociation is often reported for clusters containing as few as five water molecules, it is shown that on nanometer-sized ice nanoparticles, dissociation occurs only to a limited extent, with the majority of nitric acid remaining undissociated on the ice surface.

MO 23.2 Thu 11:30 HS XV

Imaging single sea salt aerosol nanoparticles — ●CHANGJI PAN for the Sea Salt Nanoparticle-Collaboration — Department of Physics, ETH Zurich, 8093, Zurich Switzerland

The influence of sea salt aerosol particles on atmospheric processes highly depends on their hygroscopicity and capacity as cloud condensation nuclei. These properties are highly related to the particle morphology and the distribution of chemical species inside these nanoparticles. Many studies, however, suffer from the averaging effect in ensemble measurements and the substrate interaction in deposited particles. We performed a direct measurement on in-flight individual sea salt aerosol nanoparticles by single-shot X-ray diffraction imaging at EuXFEL, to retrieve their inner structure and overall morphology as a function of particle size, chemical composition, and humidity.

MO 23.3 Thu 11:45 HS XV

Optimized sample-delivery system for coherent-diffractive-imaging of proteins — ●STEFANIE LENZEN^{1,2}, LUKAS V. HAAS^{1,3,4}, KEVIN JANSON¹, AMIT K. SAMANTA^{1,3,4}, and JOCHEN KÜPPER^{1,2,3,4} — ¹Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Chemistry, Universität Hamburg — ³Department of Physics, Universität Hamburg — ⁴Center for Ultrafast Imaging, Hamburg

Determining the structure and dynamics of single native bio-nanoparticles, such as proteins, is still challenging. Several methods, including protein-crystallography and cryo-EM, focus on this challenge, but the biomolecule needs to be fixed, which might lead to structural disintegration, and the temporal resolution of these methods are limited. X-ray free-electron lasers (XFELs) provide ultrashort pulses, enabling diffraction before destruction, and a large number of photons, promising the observation of diffraction patterns *off* single nanoparticles. Aerodynamic-lens stacks were used to deliver collimated and focused particle beams for such experiments on large nanoparticles [1]. We optimized the sample injection and extended the use of particle beams toward smaller nanoparticles and protein complexes like apoferritin. This highlights the use of improved aerosolization methods together with optimized ALS injectors for small bio-nanoparticles. In addition, we present techniques for improved optical-scattering-based detection of proteins.

[1] Lena Worbs, Toward cryogenic beams of nanoparticles and proteins, *Dissertation*, Universität Hamburg (2022)

MO 23.4 Thu 12:00 HS XV

Cryo-cooled beams of "small" macromolecules — ●JINGXUAN HE^{1,2,3}, LENA WORBS^{1,2}, SURYA KIRAN PERAVALI^{1,4}, ARMANDO D. ESTILLORE¹, AMIT K. SAMANTA^{1,3}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Physics, Universität Hamburg, Germany — ³Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany — ⁴Fakultät für Maschinenbau, Helmut-Schmidt-Universität, Germany

We demonstrated the preparation of cold and controlled beams of nanoparticles and macromolecules that are desired for x-ray single-

particle-diffractive imaging (SPI) using the buffer-gas-cell (BGC) cooling and aerodynamic focusing techniques [1,2]. The cooling and control techniques we developed for SPI can be extended to experiments to study the electron dynamics in complex biomolecules on the few-femtosecond timescale [3]. Such ultrafast charge- and energy-transfer dynamics following electronic excitation were not revealed so far [4].

We present an approach toward investigating the time-resolved ultrafast dynamics in cryo-cooled proteins [1] induced by ultrashort UV/VIS pulses and advanced detection method including velocity-map-imaging using Timepix3 cameras [5].

- [1] A.K. Samanta, *et al.*, *Struct. Dyn.* **7**, 024304 (2020)
- [2] S.K. Peravali, *et al.*, *Comput. Fluids* **279**, 106346 (2024)
- [3] M. Hervé, *et al.*, *Commun. Chem.* **4**, 124, (2021)
- [4] H. Duan, *et al.*, *PNAS* **114**, 8493 (2017)
- [5] H. Bromberger, *et al.*, *J. Phys. B* **55**, 144001 (2022)

MO 23.5 Thu 12:15 HS XV

Temperature and adsorption dynamics of single nanoparticles in a cryogenic ion trap — ●BJÖRN BASTIAN, SOPHIA C. LEIPPE, KLEOPATRA PAPAGRIGORIOU, and KNUT R. ASMIS — Wilhelm Ostwald Institute, Leipzig University, Linnéstraße 2, D-04103 Leipzig

Characterization of nanoparticles without inhomogeneous broadening and interactions with the environment requires single particle techniques in the gas phase. Our group has shown the feasibility of single nanoparticle action spectroscopy (SNAS) in a cryogenic Paul-type ion trap [1], based on the adsorption of messenger atoms or molecules on the nanoparticle surface and their desorption driven by laser heating with rates that are proportional to the absorption cross section [2].

A quantitative understanding of the sorption dependent SNAS technique and temperature programmed desorption schemes to characterize surface interactions strongly depend on the surface temperature which is difficult to measure or estimate in such experiments. In a collaborative work, we could achieve a first *in situ* measurement using the temperature-dependent emission spectrum of core/shell CdSe/CdS quantum dots and capture the essential heating and cooling processes in a model [3]. The latter helps to estimate surface temperatures for different particles and experimental conditions which is used here to interpret the adsorption dynamics of oxygen on silica nanoparticles.

[1] B. Hoffmann *et al.*, *Mol. Phys.* **122**, e2210454 (2023). [2] B. Hoffmann *et al.*, *J. Phys. Chem. Lett.* **11**, 6051 (2020). [3] S. C. Leippe *et al.*, *J. Phys. Chem. C* (accepted).

MO 23.6 Thu 12:30 HS XV

Cluster beam technologies for matter-wave interferometry — ●SEVERIN SINDELAR, BRUNO RAMIREZ-GALINDO, SEBASTIAN PEDALINO, STEFAN GERLICH, and MARKUS ARNDT — University of Vienna, Faculty of Physics, Boltzmannngasse 5, 1090 Vienna

Metal nanoparticles are promising candidates for interferometric tests of the quantum superposition principle in the 1 MDa mass range. Cluster interferometry shall allow us to push the limit on quantum macroscopicity well beyond the state of the art and it shall open a window for quantum-enhanced measurements of properties of nanoscale materials.

The cluster beam shall last for a day, have a high brilliance of slow and neutral metal nanoparticles with masses up to 1 MDa and velocities below 30 m/s. The materials must have a work function compatible with single photon ionization using deep ultraviolet (DUV) laser light, ideally high polarizability and low magnetic susceptibility. Here we present our approach to such a cluster source: It is based on metal evaporation and cluster aggregation in an 80 K cold chamber, followed by an aerodynamic lens array.

While interference experiments shall work with neutral clusters, their identification and detection require singly charged particles, which we can select in a quadrupole mass spectrometer with subsequent Daly detection. We present the formation, ionization and spectroscopy of metal clusters, which have a low work function, high absorption cross section and high polarizability. We study their photo physics as a function of size, DUV laser wavelength and laser power to extract the properties that will be needed for interference experiments.

MO 23.7 Thu 12:45 HS XV

Laser-induced alignment of macromolecules and nanoparticles — ●LUKAS VINCENT HAAS^{1,2,3}, XUEMEI CHENG¹, MUHAMED AMIN¹, STEFANIE LENZEN^{1,3}, AMIT KUMAR SAMANTA^{1,2,3}, and

JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Physics, Universität Hamburg, Germany — ³Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

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) (2021)

[2] J. C. H. Spence, et al., *Phys. Rev. Lett.* 92, 198102 (2004)

[3] M. Amin, et al., arXiv:2306.05870 [physics], (2023)

MO 23.8 Thu 13:00 HS XV

Rotational Wave Packet Dynamics of Size-selected Neutral

Clusters — •JIAYE JIN, MAX GRELLMANN, MARCEL JOREWITZ, and KNUT R. ASMIS — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Leipzig, Germany

We report our results on rotational wave-packet dynamics for the mass-selected neutral clusters in a cryogenic ion trap probed by two-colors femtosecond pump-probe spectroscopy involving the negative-neutral-positive excitation scheme. To achieve this, a rotational wave packet is prepared via photodetachment of mass-selected cold anion using a first linearly polarized laser pulse. The rotation coherence is then probed using a second linearly polarized laser pulse, set either parallel or perpendicular to the polarization of the first pulse, ionizing the neutral molecule. The rotational anisotropy β is then calculated from the cation transients probed at different polarization angles.

Neutral boron cluster B_6 is chosen as the first experimental candidate. So obtained time-dependence of B_6^+ cation measured at parallel probing polarization shows typical J-type recurrences of the initial rotational wave packet at 68 ps, 135 ps, 210 ps and 275 ps. The rotational coherence is confirmed by following measurements using perpendicular polarization, where the recurrent cations signal show opposite intensity compared to the parallel probing. An effect rotational constants is thus obtained by 0.25 cm^{-1} , agreeing well with calculations. These results demonstrate the application in the coherent control for the orientation of mass-selected neutral molecules in a cryogenic ion trap.

MO 24: Attosecond Physics II (joint session A/MO)

Time: Thursday 11:00–12:30

Location: GrHS Mathe

Invited Talk

MO 24.1 Thu 11:00 GrHS Mathe

Circular Dichroic Attosecond Transient Absorption Spectroscopy — •LAUREN DRESCHER^{1,2}, NICOLA MAYER^{2,3}, KYLIE GANNAN¹, JONAH ADELMAN¹, and STEPHEN LEONE¹ — ¹Department of Chemistry, University of California, Berkeley, California 94720, USA — ²Max-Born-Institut, Max-Born-Str. 2A, 12489, Berlin, Germany — ³Attosecond Quantum Physics Laboratory, Department of Physics, King's College London, Strand, London, WC2R 2LS, United Kingdom

The angular momentum of light couples to matter via the total angular momentum. By limiting possible orbital angular momentum states, circular polarized light can be used to enact spin-specificity onto the optical excitation of matter, even within isotropic media. We leverage this effect in our method of circular dichroic attosecond transient absorption spectroscopy to prepare and measure spin-specific coupling with attosecond temporal precision. This principle is demonstrated using co- and counter-rotating two-color excitation of helium Rydberg states, showing the effect of dipole selection and propensity rules in the selective excitation of spin-specific states. Our methods allows to study the dynamic of spin-specific excitations and gives insight into the orbital character of excited states through their interaction with circular polarized two-color fields. Furthermore we demonstrate that, given a known model system, our method allows to measure the polarization state of attosecond extreme ultraviolet (XUV) pulses in-situ and in an all-optical setup.

MO 24.2 Thu 11:30 GrHS Mathe

Attosecond Photon Diagnostics at Flash - A Dedicated Angular Streaking Beamline — •LASSE WÜLFING¹, LARS FUNKE¹, THORSTEN OTTO², SARA SAVIO¹, NICLAS WIELAND³, MARKUS ILCHEN³, and WOLFRAM HELML¹ — ¹Technische Universität Dortmund, Germany — ²Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Universität Hamburg, Germany

The established scheme of angular streaking can characterize the temporal and spectral information of ultrashort X-ray pulses non-invasively. This is done by overlapping the pulses with a circularly polarized IR laser in a gaseous target and measuring the resulting angle dependent photo electron spectra with so called *Cookiecutter*-type detectors.

We developed a new detector with optimized electron time of flight spectrometers for increased energy resolution and better overall performance. This experiment will be installed at a new diagnostics beamline at Flash 2 for a dedicated angular streaking setup.

We present an overall rundown of the experimental method and the new setup.

MO 24.3 Thu 11:45 GrHS Mathe

In Search of Lost Tunneling Time — •PABLO MAIER¹, SERGUEI PATCHKOVSKII¹, MISHA IVANOV^{1,2,3}, and OLGA SMIRNOVA^{1,4} — ¹Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Straße 2A, 12489 Berlin, Germany — ²Humboldt-Universität zu Berlin, Unter den Linden 6, 10117 Berlin, Germany — ³Solid State Institute and Physics Department, Technion, Haifa, 32000, Israel — ⁴Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

The measurement of tunneling times in strong-field ionization has been the topic of much controversy in recent years, with the attoclock and Larmor clock being two of the main contenders for correctly reproducing these times. By expressing the attoclock as the weak value of temporal delay, we extend its meaning beyond the traditional setup. This allows us to calculate the attoclock time for a static one-dimensional tunneling model consisting of a binding delta potential and a constant electric field. We apply the Steinberg weak-value interpretation of the Larmor clock. Using this definition, we obtain the position-resolved time density during tunnel ionization, yielding a non-zero Larmor tunneling time. Our model allows us to derive the analogue of the position-resolved attoclock tunneling time. While non-zero at the tunnel exit, it vanishes at the detector, far away from the atom. Formally, this means that the attoclock does not measure the Larmor time, but instead a time closely related to the phase time.

MO 24.4 Thu 12:00 GrHS Mathe

attosecond coherent control using nonlinear processes driven by a seeded FEL — •SOORAJ R.S¹, IOANNIS MAKOS¹, MICHELE DI FRAIA², OKSANA PLEKAN², PRAVEEN MAROJU³, DAVID BUSTO³, S HARTWEG¹, DAVID GARZELLA², KEVIN PRINCE², A DEMIDOVICH², JOHAN MAURITSSON³, MARVIN SCHMOLL¹, AARON NGAI¹, R MOSHAMMER⁴, C MEDINA⁴, MUWAFFAQ MOURTADA⁴, T PFEIFER⁴, TAMAS CSIZMADIA⁵, DEBOBRATA RAJAK⁵, KLEMEN BUCAR⁶, ANDREJ MIHELIC⁶, MATJAZ ZITNIK⁶, UWE THUMM⁸, FERNANDO M GARCIA⁷, CARLO CALLEGARI², ELENA GRYZLOVA¹, and GIUSEPPE SANSONE¹ — ¹Albert Ludwigs Universität Freiburg, Germany — ²Elettra Sincrotrone Trieste, Italy — ³Lund University, Sweden — ⁴MPI für Kernphysik Heidelberg, Germany — ⁵ELI ALPS, Hungary — ⁶Jožef Stefan Institute, Slovenia — ⁷Universidad Autónoma de Madrid, Spain — ⁸Kansas State University, USA

In this study, we investigate interference between two coherent pathways in two-photon double ionization (TPDI) of Ar, mediated by the $3s3p^65p$ and $3s3p^66p[1]$ states, and in N_2 through the Hopfield resonances $3d\sigma_g$ and $3d\pi_g$ [2]. Using phase-controlled XUV radiation from FEL FERMI, we record photoelectron spectra from TPDI to study how intermediate resonances affect the contrast and phase of oscil-

lations from two nonlinear-coherent paths. This study highlights the critical role of intermediate resonances in controlling the interference dynamics of multiphoton ionization processes. [1] Elena V G et al. In: The Eu Phy Jo D 73 (2019) [2] M Reduzzi et al. In: Jo of Phy B:AMO Physics 49.6 (2016)

MO 24.5 Thu 12:15 GrHS Mathe

A rigorous and universal approach for highly-oscillatory integrals in attosecond science — ●ANNE WEBER¹, JOB FELDBRUGGE², and EMILIO PISANTY¹ — ¹Attosecond Quantum Physics Laboratory, King's College London, WC2R2LS London, UK — ²Higgs 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 these 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 25: X-ray Spectroscopy

Time: Thursday 14:30–16:30

Location: HS XVI

Invited Talk

MO 25.1 Thu 14:30 HS XVI

In good neighborhood: Suppression of radiation damage to X-ray-ionized molecules by intermolecular decay — ●ANDREAS HANS¹, DANA BLOSS¹, MADHUSREE ROY CHOWDHURY¹, CATMARNA KÜSTNER-WETEKAM¹, FLORIAN TRINTER², ALEXANDER KULEFF³, LORENZ S. CEDERBAUM³, and ARNO EHRESMANN¹ — ¹Universität Kassel, Kassel, Germany — ²Fritz-Haber-Institut, Berlin, Germany — ³Universität Heidelberg, Heidelberg, Germany

The exploration of the interaction of ionizing radiation with matter is the basis of many application-related questions. In isolated small organic molecules, the deposition of energy by X-rays usually triggers complete or partial disintegration. In the transition to realistic scenarios, it is crucial how the behavior of molecules changes when they have neighbors, like in an aqueous environment. Intermolecular decays can release large amounts of energy efficiently and directly into the environment. We demonstrate that energy can already be efficiently dissipated by intermolecular Coulombic decay of electronic core vacancies. This leads to a decisive change in the dissociation dynamics of a molecule. While the dissipation of energy to the environment generally is protective for the molecule, the reverse effect can also occur, in which energy absorbed by the water leads to the ionization of a solvated molecule.

MO 25.2 Thu 15:00 HS XVI

Enhanced Intermolecular Coulombic Decay in thiophene dimers — ●DEEPTHY MARIA MOOTHERIL¹, ANNA SKITNEVSKAYA², XUEGUANG REN³, THOMAS PFEIFER¹, and ALEXANDER DORN¹ — ¹Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — ²Irkutsk, Russia — ³Xi'an Jiaotong University, Xi'an 710049, China

Inter-atomic/intermolecular Coulombic decay (ICD) is an important electronic relaxation mechanism after inner-valence ionization of atoms or molecules with weakly bound neighbours, which leads to low-energy electron emissions that can contribute to radiation damage in biological matter. In this work, we investigate ICD in thiophene dimers, five-membered aromatic ring containing sulfur, a third-row element, as a heteroatom, induced by electron collisions (68 eV). A comparison of the projectile energy loss spectra with theoretical single ionization spectra reveals that the ICD process originates from the C 2s⁻¹ inner-valence vacancy in thiophene dimers, which exhibits significant sulfur contributions. Notably, we observe that relaxation of states between the ICD and Auger thresholds results in a strong enhancement of ICD electrons below 4 eV, in contrast to other aromatic ring systems containing second-row atoms. Based on this 'ICD-only' decay contribution, we estimate a reduced relative ICD probability above the Auger threshold, where competing Auger channels become significant.

MO 25.3 Thu 15:15 HS XVI

Resonant double core hole spectroscopy of ultrafast decay dynamics in Fe complexes — ●JULIUS SCHWARZ¹, MATZ NISSEN¹, ALBERTO DE FANIS², ALJOSCHA RÖRIG², THOMAS BAUMANN², SIMON DOLD², TOMMASO MAZZA², YEVHENIY OVCHARENKO², SERGEY USENKO², ANDREAS PRZYSTAWIK^{1,6}, KAROLIN BAEV⁵, HAMPUS WIKMARK³, FLORIAN TRINTER⁴, TIM LAARMANN^{1,6}, MARKUS ILCHEN^{1,2}, NILS HUSE¹, MICHAEL MEYER², PHILIPPE VERNET³,

and MICHAEL MARTINS¹ — ¹Universität Hamburg, Germany — ²European XFEL, Hamburg, Germany — ³Uppsala University, Sweden — ⁴Fritz-Haber-Institut, Berlin, Germany — ⁵DESY, Hamburg, Germany — ⁶The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Resonant double core hole (DCH) spectroscopy allows for the observation of ultrafast dynamic processes in small 3d-metal compounds in the gas phase with enhanced sensitivity. Using the intense X-Ray pulses of the European XFEL, electron and ion spectroscopy was used to reveal the signature of iron 2p² resonant DCH excitation in iron pentacarbonyl and ferrocene. Comparing the experimental results to theoretical calculations reconstructs single core hole (SCH) and DCH photon-matter interactions in the two targets. The DCH Auger-Meitner electron signals offer insight to the electron dynamics during the core hole lifetime and their dependence on the chemical environment. The product ions show evidence for DCH processes in multiply charged iron cations.

MO 25.4 Thu 15:30 HS XVI

XUV Double-Ionisation of Micro-Solvated Bio-relevant Molecules — ●BRENDAN WOUTERLOOD¹, SITANATH MONDAL¹, MYRIAM DRISSI², MADHUSREE ROY-CHOWDHURY², GUSTAVO GARCIA-MARCÍAS², LAURENT NAHON², FRANK STIENKEMEIER¹, and SEBASTIAN HARTWEG¹ — ¹Institute of Physics, University of Freiburg — ²Synchrotron SOLEIL, St. Aubin, France

Studying the XUV-photoionisation of biomolecules, 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 such as electron-ion coincidence spectroscopy. The electron-ion-ion coincidence detection of doubly-ionised molecules and complexes enables correlation of cationic states to certain fragmentation pathways. Above the double-ionisation potential, molecular fragmentation channels differ from single ionisation processes with intramolecular proton transfer reactions stabilising the cationic fragments. In these complexes different auto-ionisation processes, such as the non-local intermolecular Coulombic decay (ICD) and electron transfer mediated decay (ETMD), and local Auger-Meitner decay can thus be distinguished. These processes are important to the field of radiation chemistry since the production of low energy electrons can trigger reactions which damage biological material.

MO 25.5 Thu 15:45 HS XVI

Influence of a single water molecule on the X-ray absorption spectra of gas-phase phosphotyrosine — ●JULIETTE LEROUX^{1,2,3}, JEAN-YVES CHESNEL¹, LUCAS SCHWOB², and SADIA BARI^{2,4} — ¹CIMAP, University of Caen — ²Deutsches Elektronen-Synchrotron DESY — ³University of Hamburg — ⁴University of Groningen

The isolation of biomolecules in the gas phase removes all interactions with the solvent and enables stepwise control of these interactions by

progressively increasing the number of bound water molecules, ultimately bridging the gap between isolated molecules and aqueous conditions. Already, a single water molecule can induce significant structural changes in the molecule, such as the location of the protonation site. Over the last thirty years, there have been efforts to develop experimental techniques to study hydrated species in the gas phase using an electrospray ionization source.

To study the effect of hydration on the structure of biomolecules, our technique of choice is near-edge X-ray absorption mass spectrometry (NEXAMS). NEXAMS provides a local probe into the atomic environment and is based on the electronic excitations of core electrons to unoccupied molecular orbitals, thus capturing the electronic and geometric structure of the system under investigation. In this context, we studied the influence of a single water molecule on the structure and radiation-induced fragmentation of protonated phosphotyrosine. In particular, I will discuss the results we obtained at the carbon and oxygen K-edges in comparison with density functional theory calculations to decipher the structure of singly hydrated phosphotyrosine.

MO 25.6 Thu 16:00 HS XVI

Ultrafast molecular ion dynamics illuminated by soft X-ray spectroscopy — ●SIMON REINWARDT¹, ALEXANDER PERRY-SASSMANNSHAUSEN², TICIA BUHR³, ALFRED MÜLLER², STEFAN SCHIPPERS², FLORIAN TRINTER⁴, and MICHAEL MARTINS¹ — ¹Universität Hamburg, Hamburg, Germany — ²Justus-Liebig-Universität Gießen, Gießen, Germany — ³Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ⁴Fritz-Haber-Institut, Berlin, Germany

Synchrotron radiation has turned out to be a very powerful tool to study molecular dynamics of small molecules [1]. Photoexcitation is an instructive technique that facilitates the investigation of ultrafast dissociation processes on a time scale similar to lifetime of Auger decay [2]. Using the photon-ion merged-beams technique, implemented

at the Photon-Ion Spectrometer at PETRA III (DESY, Hamburg), we measured the kinetic energy release of molecular ions depending on the photon energy [3]. Thereby, the ultrafast dynamics of the photodissociation process of molecular ions NH^+ and OH^+ was revealed particularly as a result of $1s \rightarrow \pi^*$ and $1s \rightarrow \sigma^*$ excitations.

- [1] J. D. Bozek and C. Miron, *J. Electron. Spectrosc. Relat. Phenom.* **204**, 269 (2015).
- [2] O. Travnikova *et al.*, *Phys. Rev. Lett.* **116**, 213001 (2016).
- [3] M. Martins *et al.*, *J. Phys. Chem. Lett.* **12**, 1390 (2021).

MO 25.7 Thu 16:15 HS XVI

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, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

A newly developed apparatus enables X-ray photoelectron spectroscopy on mass-selected cluster ions at synchrotrons for the first time. The system's centerpiece is a liquid nitrogen-cooled linear Paul trap, where stored cluster ions interact with synchrotron radiation. The emitted electrons are directed by a specially designed magnetic field into a Hemispherical Energy Analyzer, where photoelectron spectra are captured. Clusters are generated in a magnetron cluster source, mass-selected using a quadrupole mass spectrometer, and then introduced into the linear ion trap. This setup enables element-specific binding energy measurements of core levels, providing detailed insights into the chemical bonding of pure and mixed metal and semiconductor clusters. Additionally, we will present initial test spectra of emitted electrons recorded with the apparatus, demonstrating its ability to capture high-resolution photoelectron spectra and validating its potential for advancing studies in cluster ion chemistry and bonding.

MO 26: Poster – Cold Molecules (joint session MO/Q)

Time: Thursday 17:00–19:00

Location: Tent

MO 26.1 Thu 17:00 Tent

Delta-Kick Collimation of Heteronuclear Feshbach Molecules — ●TIMOTHÉ ESTRAMPES^{1,2}, JOSE P. D'INCAO^{3,4}, JASON R. WILLIAMS⁵, ÉRIC CHARRON², and NACEUR GAALOU¹ — ¹Leibniz University Hannover, Institut für Quantenoptik, Germany — ²Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, France — ³JILA, NIST, and the Department of Physics, University of Colorado, Boulder, CO 80309, USA — ⁴Department of Physics, University of Massachusetts Boston, Boston, MA 02125, USA — ⁵Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA

Delta-Kick Collimation [Phys. Rev. Lett. 78, 2088 (1997)] is a well-known process in atomic physics that allows to drastically reduce the expansion energy of a cold sample by flashing an external potential during its release. Here, we theoretically explore the extension of this process to cold heteronuclear Feshbach molecules.

We first investigate the validity of neglecting the coupling between the center-of-mass motion and molecular vibrations. After establishing the domain of validity for this approximation, we use scaling approaches to estimate the achievable gains over a large range of temperature and density regimes. For typical external trap parameters, the expansion energy of a thermal cloud could be reduced by a factor of 100, increasing to over 500 for a heteronuclear condensed molecule.

MO 26.2 Thu 17:00 Tent

Photoassociation Spectroscopy of RbYb near the Yb intercombination line — ●CÉLINE CASTOR, CHRISTIAN SILLUS, ARNE KALLWEIT, and AXEL GÖRLITZ — Uni 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 first experiments in our apparatus for the production of ultracold RbYb molecules. This setup constitutes an improvement of our old apparatus, where the interactions in RbYb and possible routes to molecule production have already been studied extensively. In the new setup a major goal is the efficient production of ground

state RbYb molecules. We employ optical tweezers to transport individually cooled samples of Rb and Yb from their separate production chambers to a dedicated science chamber. Here we start to study interspecies interactions of different isotopes by overlapping crossed optical dipole traps. To explore the pathways towards ground state molecules we start with photoassociation spectroscopy near the intercombination line of Yb.

MO 26.3 Thu 17:00 Tent

Casimir-Polder Force in a Nonlinear Medium — ●NICOLAS SCHÜLER, OMAR JESÚS FRANCA SANTIAGO, and STEFAN YOSHI BUHMANN — Institut für Physik, Universität Kassel

The discovery of the Casimir effect in 1948 [1] has, among others, created a new research field involving vacuum forces and fluctuations. The Casimir effect gives rise to the attractive Casimir force [2] between two neutral polarizable bodies in vacuum as well as to the Casimir-Polder force between a particle and a polarizable macroscopic body. In our work, we theoretically investigate the latter for a chiral molecule with three crossed electric dipole transitions. In order for these purely electric contributions to give rise to a chiral force, we consider the interaction with a chiral nonlinear medium. Using macroscopic quantum electrodynamics [3,4], we analytically calculate the resulting energy correction in third order perturbation theory as well as the Casimir-Polder force between an atom in its ground state and the field.

- [1] Casimir, H. B. G.: On the attraction between two perfectly conducting plates, Proc. K. Ned. Akad. Wet. 51, 793 (1948)
- [2] Casimir, H. B. G., Polder, D.: The influence of Retardation on the London-van der Waals Forces, Phys. Rev. 73, 4 (1948)
- [3] Buhmann, S. Y.: Dispersion Forces I. Macroscopic Quantum Electrodynamics and Ground-State Casimir, Casimir-Polder and van der Waals Forces. (Springer, Berlin Heidelberg, 2012)
- [4] Lindel, F., Bennett, R., Buhmann, S. Y.: Phys. Rev. A 102, 041701(R) (2020)

MO 26.4 Thu 17:00 Tent

Technology for spatially resolved spectroscopy of Ryd-

berg states in nitric oxide — ●HANNA LIPPMANN¹, YANNICK SCHELLANDER², FABIAN MUNKES¹, ALEXANDER TRACHTMANN¹, FLORIAN ANSCHUTZ¹, ETTORE EDER¹, MERIEM MAVLUTOVA¹, ROBERT LÖW¹, PATRICK SCHALBERGER², NORBERT FRUEHAUF², HARALD KÜBLER¹, and TILMANN PFAU¹ — ¹5th Institute of Physics, University of Stuttgart, Germany — ²Institute for Large Area Microelectronics, University of Stuttgart, Germany

High-resolution continuous-wave (cw) laser spectroscopy of nitric oxide (NO) molecules has been performed to study and characterize the energy-level structure. Special focus is on effects of electric fields on high Rydberg states. In contrast to theory, the measurements show states with no frequency shift. The reason for this effect is most likely an inhomogeneous electric field distribution. This is caused by field attenuations near the cell walls resulting from charge carrier accumulations on these. Therefore, Rydberg states near the cell walls experience a much lower electric field than expected. To further investigate the charge carrier effects and prove the given explanation, spatially resolved measurements of the ionization currents are performed. These kinds of measurements are enabled by an electrode / transimpedance amplifier array based on thin-film technology. The focus is on the creation of current to voltage converting circuits using amorphous indium gallium zinc oxide as semiconductor. The same technology can be used to efficiently detect the ground state transition laser or uv light in general.

MO 26.5 Thu 17:00 Tent

Towards cavity-control of a molecular quantum gas — JOHANNES SEIFERT, MARIAN DUERBECK, NELSON WERUM, LENNARD REIHS, DALILA ROBLEDO, JUAN PABLO MARULANDA, GERARD MEIJER, and ●GIACOMO VALTOLINA — Faradayweg 4-6, 14195 Berlin

We report on a new experimental apparatus for the creation of a dipolar quantum gas of atoms and molecules inside an high-finesse optical cavity. By coupling light to matter, we want to create and control new emergent particles, so-called molecular polaritons, that can display a different chemical reactivity with respect to the original system and use them to control chemical reactions at ultracold temperatures.

MO 26.6 Thu 17:00 Tent

Towards an ultracold Fermi gas of ${}^6\text{Li}{}^{87}\text{Rb}$ molecules — ●XINYI HUANG^{1,2}, YUNXUAN LU^{1,2}, ANWEI ZHU^{1,2}, CHENHAO NI^{1,2}, and XINYU LUO^{1,3} — ¹Max Planck Institute of Quantum Optics — ²Ludwig Maximilian University of Munich — ³Munich Center for Quantum Science and Technology

We present progress on developing a new setup for producing a Fermi gas of ${}^6\text{Li}{}^{87}\text{Rb}$. Our next-generation ultracold alkali polar molecule apparatus features a compact vacuum design and rapid cycling time. By incorporating a short-range lithium Zeeman slower into the 2D magneto-optical traps (MOT) for two species in series, we achieve an atomic loading rate of 1×10^{10} atoms/s for ${}^6\text{Li}$ and 6×10^8 atoms/s for ${}^{87}\text{Rb}$, promising an excellent starting point for the rapid production of double-degenerate lithium-rubidium atomic mixtures. Additionally, we discuss theoretical predictions and experimental proposals for stimulated Raman adiabatic passage (STIRAP) of LiRb molecules to the vibrational ground state, a critical step in preparing a deeply degenerate Fermi gas of LiRb molecules.

MO 26.7 Thu 17:00 Tent

Construction of a cryogenic buffer gas source for slow, cold molecular beams — ●NICK VOGLEY¹, BERND BAUERHENNE², DANNY GEORGE¹, SIMON SCHÖPS¹, and DAQING WANG¹ — ¹Institut für angewandte Physik, Universität Bonn, Bonn, Germany — ²Institut für Physik, Universität Kassel, Kassel, Germany

We report on the construction of a cryogenic buffer gas beam source operating with helium reservoir pressure $P_0 \approx 10$ Pa and high throughput $J \approx 20$ sccm at $T_0 = 4$ K. This opens the possibility to work with higher molecular sample densities compared to the more conventional $P_0 < 0.1$ Pa machines present. The higher density also implies more efficient thermalization at a potentially increased rate of helium-molecule cluster formation, which may be investigated separately. We simulated the performance of this design in the hydrodynamic regime with a combination of computational fluid dynamics (CFD) and direct simulation Monte-Carlo (DSMC).

MO 26.8 Thu 17:00 Tent

Collisions in a quantum gas of bosonic ${}^{23}\text{Na}{}^{39}\text{K}$ molecules — ●MARA MEYER ZUM ALTEN BORGLOH¹, JULE HEIER¹, PHILIPP

GERSEMA¹, KAI KONRAD VOGES³, CHARBEL KARAM², OLIVIER DULIEU², LEON KARPA¹, and SILKE OSPELKAUS¹ — ¹Leibniz Universität Hannover, Institut für Quantenoptik — ²Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton — ³Centre for Cold Matter, Blackett Laboratory, Imperial College London

We present our experiments with quantum gases of polar ${}^{23}\text{Na}{}^{39}\text{K}$ molecules, discussing both atom-molecule and molecule-molecule collisions. In particular, we investigate the origins of loss processes in a cloud of chemically stable molecules and share our observations of magnetically tunable resonances between NaK and K. Furthermore, we outline a method for suppressing molecular loss by using a coherent two-photon transition to create a potential barrier, which prevents the colliding molecules from reaching the short-range.

MO 26.9 Thu 17:00 Tent

Merged-beams study of HD^+ with ground-term C Atoms reveals intramolecular kinetic isotope effect. — ●L. BERGER¹, F. GRUSSIE¹, M. GRIESER¹, Á KÁLOSI^{2,1}, D. MÜLLER¹, O. NOVOTNÝ¹, A. ZNOTINS¹, F. DAYOU³, X. URBAIN⁴, and H. KRECKEL¹ — ¹Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — ²Columbia Astrophysics Laboratory, Columbia University, New York 10027, USA — ³Sorbonne Université, Observatoire de Paris, PSL University, CNRS, LERMA, F-92195 Meudon, France — ⁴Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, B-1248 Belgium

The reaction of HD^+ and ground-state C atoms has been studied in a merged-beams experiment at the Cryogenic Storage Ring (CSR) of the Max Planck Institute for Nuclear Physics in Heidelberg. The CSR is cooled by a closed-cycle liquid helium unit, thus reducing the blackbody radiation field strongly compared to room-temperature experiments. HD^+ is stored for up to 20 s in the CSR and cools radiatively to the vibrational ground state (within 0.5 s) and rotational states with $J \leq 3$ (after 5 s). In contrast to previous studies with internally excited H_2^+ and D_2^+ reacting with C, a significant increase in the absolute rate coefficient of the reaction is observed and the production of CH^+ is favored over CD^+ across all collision energies. Our experimental results agree well with our quasiclassical trajectory calculations based on two reactive potential energy surfaces for vibrationally relaxed HD^+ in its lowest rotational states. [1] F. Grussie, et al. Phys. Rev. Lett. 2024, 132.243001 [2] F. Grussie, et al. Phys. Rev. A 2024, 109.062804

MO 26.10 Thu 17:00 Tent

Two Robust Methods for Extracting an Electric-Field Distribution from Microwave Depletion Spectra — ●PHILIPP HEINRICH, FLORIAN JUNG, JINDARATSAMEE PHROMPAO, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany

Electrically trapped polyatomic polar molecules can be employed in a wide range of experiments, such as in the study of collisions, spectroscopy, and cooling. Towards this end, precise knowledge of the distribution of electric fields inside the trap is indispensable, because it determines spectroscopic lineshapes when driving microwave transitions. Thus, determining the electric-field distribution from spectroscopy measurements should be possible. However, a direct extraction of this property is rendered difficult, as in general more than one transition is resonant with a certain microwave frequency at different points inside the trap, i.e. in different electric fields.

Here, we present two robust and generic strategies to resolve this problem, each employing a different microwave transition. Microwave depletion spectra are obtained inside an electrostatic multipole trap using cold CH_3F molecules loaded from a cryofuge source [1]. From those, the electric-field distribution in the trap is deduced and shown to be in good agreement with a simulated distribution. We discuss how the results obtained can be generalized to other types of electrostatic traps.

[1] M. Koller *et al.*, Phys. Rev. Lett. **128**, 203401 (2022).

MO 26.11 Thu 17:00 Tent

Towards p-wave superfluids of microwave-shielded fermionic NaK molecules — ●WEIKUN TIAN^{1,2}, SHRESTHA BISWAS^{1,2}, SEBASTIAN EPELT^{1,2}, XINGYAN CHEN^{1,2}, CHRISTINE FRANK^{1,2}, IMMANUEL BLOCH^{1,2,3}, and XINYU LUO^{1,2} — ¹Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — ²Munich Center for Quantum Science and Technology, 80799 Munich, Germany — ³Fakultät für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany

Degenerate quantum gases with long-range dipolar interactions open

exciting opportunities to explore exotic quantum phases and the dynamics of quantum many-body systems. Ultracold polar molecules, in particular, provide a promising platform to realize these phases, including topological dipolar p-wave superfluidity.

In this poster, we present our recent progress in achieving precise control over the dipolar interactions of NaK molecules through microwave dressing. This technique enables us to engineer the shape and symmetry of the intermolecular potential, suppress inelastic collisions, and perform evaporative cooling to reach the deeply degenerate regime. We highlight the development of a high-power, ultra-low-phase-noise microwave system that facilitates double-microwave dressing and supports our progress toward realizing a p-wave superfluid with dipolar BCS pairing. These advancements pave the way towards uncovering novel quantum phases in dipolar systems.

MO 26.12 Thu 17:00 Tent

Advancements towards Zeeman slowing and trapping of CaF — ●TIMO POLL, JULIUS NIEDERSTUCKE, SEBASTIAN ANSKEIT, MARIAH STEPANOVA, PAUL KAEBERT, SUPENG XU, MIRCO SIERCKE, and SILKE OSPELKAUS — Institut für Quantenoptik, Leibniz Universität Hannover

Significant advancements have recently been achieved in direct laser cooling of molecules, bringing them to temperatures near absolute zero [1,2]. Nevertheless, the number of molecules that can be trapped from molecular beams using standard laser-based techniques remains a limiting factor in experiments [3,4]. In this work, we explain our strategies to enhance the molecular yield in these experiments. We present our experimental findings on the Zeeman slower developed for directly laser-coolable molecules, as proposed by our group [5], alongside the concepts and initial experimental efforts aimed at establishing a sub-Doppler cooling 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. 2018
- [5] M. Petzold et al. 2018
- [6] S. Xu et al. 2021
- [7] S. Xu et al. 2022

MO 26.13 Thu 17:00 Tent

Towards magneto-optical trapping of molecules in the deep ultraviolet — ●LAJOS PALANKI¹, JIONGHAO CAI², CARLOS ALARCON-ROBLEDO¹, CALEB RICH¹, WEI WEI LIU¹, JOSÉ EDUARDO PADILLA-CASTILLO², RUSSEL THOMAS², GERARD MEIJER², SIDNEY WRIGHT², and STEFAN TRUPPE^{1,2} — ¹Centre for Cold Matter, Imperial College London — ²Fritz Haber Institute, Berlin

In recent years, ultracold molecules have become a very promising platform for quantum information processing, studying quantum many-body physics and testing new physics beyond the Standard Model of particle physics.

Similar to alkaline earth (like) atoms (Yb, Sr, Cd) aluminium monofluoride (AlF), has a strong dipole-allowed transition (near 227.5 nm) to capture and cool a large number of molecules in a MOT and narrow spin-forbidden transitions for cooling to low temperatures in the μ K range. This might allow trapping laser-cooled molecules at high enough densities to study collisions between the molecules and evaporative cooling to form a degenerate gas of polar molecules.

We present a new laser system based on Vertical External Cavity

Surface Emitting Lasers (VECSELs) to generate high-power DUV light for laser cooling. We demonstrate its versatility by characterising the molecular source to produce an intense beam of AlF molecules and by capturing and cooling Cd atoms in a magneto-optical trap.

MO 26.14 Thu 17:00 Tent

Deep ultraviolet laser cooling of cadmium atoms and AlF molecules — ●E. PADILLA¹, J. CAI¹, S. HOFSSÄSS¹, L. PALANKI², R. THOMAS¹, S. KRAY¹, B. SARTAKOV¹, G. MEIJER¹, S. TRUPPE², and S. WRIGHT¹ — ¹Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — ²CCM, Imperial, SW7 2AZ London, UK

Aluminium monofluoride (AlF) is a promising candidate for laser cooling and trapping at high densities. The primary laser cooling transition at 227.5 nm is extremely strong, highly vibrationally diagonal, and it is feasible to slow a molecular beam from 200 m/s to rest in 10 cm.

Since deep ultraviolet laser technology remains challenging, we first tested our experimental setup with a simple atomic system. The principal singlet-singlet transition from the electronic ground state in Cd, analogous to the laser cooling transition in AlF, lies conveniently near in wavelength at 229 nm. We demonstrate chirped frequency laser slowing on this transition using a buffer gas cooled Cd atomic beam, and load these atoms into a magneto-optical trap (MOT).

To study the efficacy of laser slowing AlF, we apply the pump-probe time-of-flight velocity measurement technique presented in [1]. This method relies only on rapid optical pumping of molecules between rotational levels of the electronic ground state, and allows efficiently measuring the velocity distribution in any rotational state. Applying chirped frequency laser slowing, we are able to slow molecules from 150 m/s to below 40 m/s in three different rotational states. This is the expected capture velocity of a molecular MOT of AlF.

- [1] S Hofsäss *et al* 2021 *New J. Phys.* **23** 075001

MO 26.15 Thu 17:00 Tent

Experiments with continuous sources of AlF molecules — ●PRIYANSH AGARWAL¹, SIDNEY WRIGHT¹, PULKIT KUKREJA¹, EDUARDO PADILLA¹, MAXIMILIAN DOPPELBAUER¹, RUSSELL THOMAS¹, XIANGYUE LIU¹, SEBASTIAN KRAY¹, JIONGHAO CAI², BORIS SARTAKOV¹, STEFAN TRUPPE², and GERARD MEIJER¹ — ¹Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — ²Imperial College London, Exhibition Rd, South Kensington, London SW7 2AZ

The AlF molecule, subject to laser cooling and trapping efforts, has the advantage that it can be efficiently produced by a thermochemical reaction. Here we present a series of experiments on continuous molecular beam sources of AlF, primarily using the reaction between aluminium metal and aluminium trifluoride vapour. We compare a compact AlF molecular beam oven operating near 900 K to a pulsed, laser ablation-based supersonic molecular beam. The continuous, far-field flux from the oven begins to exceed the peak brightness from the supersonic source for the $v = 0, J = 7$ level, and we show that an excellent signal-to-noise ratio can be obtained for high rotational levels in pulsed laser ionisation experiments. By injecting flux from the oven output into a cryogenic buffer gas cell, we cool the internal temperature to around 30 K and reduce the most probable forward velocity from 700 m/s to 260 m/s using Neon buffer gas. Furthermore, we demonstrate a molecular dispenser source, wherein the molecules thermalise to the laboratory temperature via collisions with vacuum walls of the experiment, generating a room temperature transient molecular vapour.

MO 27: Poster – Collisions, Scattering and Correlation Phenomena (joint session A/MO)

Time: Thursday 17:00–19:00

Location: Tent

MO 27.1 Thu 17:00 Tent

Light-induced correlations in cold dysprosium atoms — ●CHUNG-MING HUNG, ISHAN VARMA, MARVIN PROSKE, RHUTHWIK SRIRANGA, DIMITRA CRISTEA, and PATRICK WINDPASSINGER — Institut für Physik, Johannes Gutenberg Universität Mainz

When the average atomic distance in a cloud of ultracold atoms, is below the wavelength of the scattering light, a direct matter-matter coupling is introduced by electric and magnetic interactions. This alters the spectral and temporal response of the sample, where the atoms cannot be treated as individual emitters anymore. We intend

to experimentally study light-matter interactions in dense dipolar media with large magnetic moments to explore the impact of magnetic dipole-dipole interactions on the cooperative response of the sample. With the largest ground-state magnetic moment in the periodic table (10 Bohr-magneton), dysprosium is the perfect choice for these experiments. This poster reports on the progress in generating dense, cold dysprosium clouds. We discuss the measures taken to optically transport the atoms into a home-built science cell by utilizing an air-bearing translation stage. The cell compact design allows for tight dipole trapping with a high numerical aperture objective. Finally, an outlook is provided on future measurements aimed at the collective response in

the generated sample.

MO 27.2 Thu 17:00 Tent

Electron Capture Dynamics and Momentum Reconstruction in Ion-Neutral Collisions of Molecular Oxygen Using the Trap-REMI — ●CRISTIAN MEDINA and HENRI LURTZ — Saupfercheckweg 1, 69117 Heidelberg

We present the momentum reconstruction and Q-value of ion-neutral collisions involving molecular oxygen ($O_2^+ - O_2^*$). Coincidence measurements were performed using the Trap-REMI setup, which combines reaction microscopy (REMI) with an electrostatic ion beam trap. This configuration enables collisions between stored ion species and a neutral gas jet. For the first time, we provide a complete description of a molecular collision using this setup, advancing toward coincidence measurements of electron/ion/neutral products.

In addition, we analyzed ion bunch dynamics, mass spectrometry of the collision products, and its velocity distributions. The results primarily indicate an electron capture process, transferring an electron from the neutral molecule to the ion. These findings offer valuable insights into ion-neutral collision dynamics and lay the groundwork for extending the method to systems of higher complexity that have significant implications for molecular physics, astrophysics, and atmospheric

studies. measurements

MO 27.3 Thu 17:00 Tent

About Ion-neutral coincidence measurements on $O_2-O_2^+$ collisions using the Trap-REMI — ●HENRI LURTZ — Max Planck Institute of Nuclear Physics, Heidelberg, Germany

We present the study of ion-neutral collisions involving molecular oxygen ($O_2^+ - O_2$) using the Trap-REMI setup. This apparatus integrates reaction microscopy (REMI) with electrostatic ion beam trapping, enabling coincidence measurements between stored ion species and a neutral gas jet. We report on the optimization of ion trap simulations, experimental setup refinements, and the characterization of a new electron cyclotron resonance (ECR) ion source. Additionally, we analyzed ion bunch dynamics, mass spectrometry of collision products, and velocity distributions from coincidence measurements. The results primarily indicate an electron capture process, transferring an electron from the neutral molecule to the ion. Furthermore, a novel bunch-splitting mechanism was observed at extended trapping times, attributed to the high space charge ratio within the ion bunch. These findings contribute valuable insights into ion-neutral collision dynamics and have implications for understanding molecular oxygen processes in astrophysics and atmospheric physics.

MO 28: Ultrafast Dynamics IV

Time: Friday 11:00–12:45

Location: HS XVI

MO 28.1 Fri 11:00 HS XVI

Generation of atomic coherence by ultrafast molecular photodissociation probed by heterodyned detected attosecond four-wave-mixing spectroscopy — ●FRANCESCO MONTORSI^{1,2}, PATRICK RUPPRECHT³, LEI XU⁴, NIRI GOVIND⁴, SHAUL MUKAMEL⁵, MARCO GARAVELLI², DANIEL M. NEUMARK³, STEPHEN R. LEONE³, and DANIEL KEEFER¹ — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²Dipartimento di Chimica industriale Toso Montanari, Università di Bologna, 40136 Bologna, Italy — ³Department of Chemistry, University of California, Berkeley, California 94720, USA — ⁴Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352, United States — ⁵Department of Chemistry, Physics and Astronomy, University of California, Irvine, California 92697, USA

Electronic coherences (EC) in molecules can naturally form, after photoexcitation, in the vicinity of so-called conical intersections (CIs). Here, we theoretically investigate the evolution of EC generated during a photochemical process namely the bond cleavage in methyl iodine. Quantum dynamics simulations show that the coherence spawned in the molecule by a CI is rapidly transferred to the atomic iodine upon dissociation. This allows the preparation of a long-lived EC, making it interesting for quantum technology applications. Finally, we propose a spectroscopic scheme based on the interference of two attosecond four-wave mixing signals which enables a background-free tomography of such EC providing crucial information about its generation at the molecular CI

MO 28.2 Fri 11:15 HS XVI

Absolute Photoemission Timing of Surface-Oriented Iodoalkanes on Pt(111) — PASCAL FREISINGER¹, ●SVEN-JOACHIM PAUL¹, CHRISTIAN SCHRÖDER², KONSTANTIN SEIDENFUS¹, PETER FEULNER³, and REINHARD KIENBERGER¹ — ¹Chair for laser and x-ray physics, E11, Technische Universität München, Germany — ²University of California, Berkeley, USA — ³Surface and Interface Physics, E20, Technische Universität München, Germany

We report on attosecond streaking measurements of the electron photoemission process from the platinum (111) surface covered by surface-oriented iodoalkanes. Attosecond streaking enables measuring relative time delays in photoemission from two energetically different bound electronic states. This experiment investigated how the photoemission delay between the platinum valence band and the iodine 4d state in iodomethane, iodoethane, and atomic iodine depends on surface coverage.

Both Iodoalkanes align horizontally or vertically to the Pt(111) surface, depending on coverage. Therefore, changing the surface coverage changes the surface orientation of adsorbed iodomethane or iodoethane, thus enabling measuring photoemission delays under a fixed

emission angle. This overcomes common attosecond streaking experiments in the gas phase, where the photoemission delay is averaged over the full solid angle.

Streaking atomic iodine enables referencing an established timing scheme in the gas phase, making retrieved photoemission delays comparable to gas phase measurements.

MO 28.3 Fri 11:30 HS XVI

Time resolved attosecond photoemission of isosteric molecules — ●MAXIMILIAN POLLANKA¹, CHRISTIAN SCHRÖDER¹, MAXIMILIAN FORSTER¹, PASCAL FREISINGER¹, SVEN-JOACHIM PAUL¹, ZDENEK MASIN², JAKUB BENDA², and REINHARD KIENBERGER¹ — ¹Physik-Department, Technische Universität München, Garching, Germany — ²Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

In this work we report on the absolute photoemission timing of the outer valence states in the isosteric molecules CO₂ and N₂O utilizing attosecond streaking spectroscopy. We investigated on the photon energy dependant emission times using helium and iodomethane as a timing reference. Employing the time-dependant R-matrix approach, the channel-coupling effect turned out to be a significant delay contribution in CO₂ due to the resonant coupling of the NIR field with the B and C states separated by 1.3 eV. Based on the theoretical calculations we could disentangle the respective delay contribution of single states in an experimentally accessible mixed state, where in both molecules the II orbital turned out to be the dominant electron supplier. By comparing the absolute photoemission times retrieved with both chronoscopes He and CH₃I, we could proof the validity of using HeI_s as well as I4d as complementary reference photolines. The great agreement of the absolute delays obtained with both timing references make us confident for further exploiting the I4d in prospective absolute timing experiments of outer valence states in molecules.

MO 28.4 Fri 11:45 HS XVI

Asymmetry parameter of the iodoalkanes — ●MAXIMILIAN FORSTER¹, MAXIMILIAN POLLANKA¹, SVEN-JOACHIM PAUL¹, PASCAL FREISINGER¹, CHRISTIAN SCHRÖDER¹, MICHELE ALAGIA², ALESSIO BRUNO³, ROBERT RICHTER², STEFANO STRANGES³, and REINHARD KIENBERGER¹ — ¹Technische Universität München — ²Elettra Synchrotron Trieste — ³Sapienza University of Rome

We measured the asymmetry parameter of photoemission from the Iodine 4d state in four different Iodoalkanes across an energy range of 60 to 160 eV.

We previously conducted photoemission delay measurements of the Iodoalkanes in our group using attosecond streaking. There we see a dependence on the species, the molecular surrounding of the iodine atom influences its photoemission delay. Since photoemission delay is interpreted as scattering delay, intramolecular scattering of the out-

going photoelectron is a logical explanation. It has been shown experimentally that the molecular environment can affect the asymmetry parameter, most likely also through intramolecular scattering. By measuring the asymmetry parameter we can compare the behavior to our previous measurements and clearly identify intramolecular scattering as the underlying cause for the behavior both in the time and the spectral domain. While we saw an effect, it is not the same as in our measurements, therefore the picture is not as intuitive as we had hoped.

The measurements were conducted at the Elettra synchrotron using the gas phase endstation.

MO 28.5 Fri 12:00 HS XVI

Time- and energy-resolved fluorescence measurements of collective effects in organic aggregates attached to rare gas clusters — ●ALEKSANDR DEMIANENKO, MORITZ MICHELBAACH, SEBASTIAN HARTWEG, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

Collective effects in organic semiconductors affect excited state lifetimes, important for organic optoelectronic and photovoltaic applications. A complete understanding of the energy level structure, and decay mechanisms require high spectral and temporal resolution. We present a setup combining conventional laser-induced fluorescence (LIF) spectroscopy with time-correlated single photon counting (TC-SPC) and discuss advantages and implementation challenges. Using wavelength-tunable nanosecond dye laser pulses allows us to measure high-resolution LIF spectra of transitions to highly excited states of tetracene embedded in superfluid helium nanodroplets, or deposited on solid rare-gas clusters. The newly implemented TCSPC detection in combination with a femtosecond laser system is aimed at studying radiative and non-radiative decay mechanisms connected to collective effects in aggregates of polyacenes. This technique allows us to cover the sub-ns lifetime region not previously reachable in our fluorescence measurements.

MO 28.6 Fri 12:15 HS XVI

A systematic study of vibrational decoherence of PTCDA in different environments using two-dimensional electronic spectroscopy — ●YILIN LI, ARNE MORLOK, ULRICH BANGERT,

JAKOB GERLACH, BRENDAN WOUTERLOOD, FRANK STIENKEMEIER, and LUKAS BRUDER — Institute of Physics, University of Freiburg, Germany

We present a systematic study of the coupling and energy dissipation of vibrational modes in different environments, ranging from cold isolated molecules in the gas phase, to molecules embedded in different rare-gas cluster species and molecules dissolved in a solution at room temperature. As test molecule we chose 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) and apply femtosecond pump probe and two-dimensional electronic spectroscopy (2DES) [1,2]. This approach provides insight into the various aspects of vibrational decoherence, e.g. pure dephasing processes and energy dissipation into the environment, and can be applied in all environments, allowing for a direct comparison of the experimental results.

1. L. Bruder et al., Nat. Commun. (2018), 9, 4823

2. U. Bangert, F. Stienkemeier, L. Bruder, Nat. Commun. (2022), 13, 3350

MO 28.7 Fri 12:30 HS XVI

Anomalous diffusion of free-base phthalocyanine on rare-gas clusters — ●ARNE MORLOK, ULRICH BANGERT, PHILIPP ELSÄSSER, YILIN LI, FELIX RIEDEL, TANJA SCHILLING, LUKAS BRUDER, and FRANK STIENKEMEIER — University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Precise knowledge and control of the environment are essential in diffusion studies, as interactions between a diffusing particle and its surroundings can lead to anomalous diffusion, deviating from simple Brownian motion. To address this, we employ cluster-isolation spectroscopy, which provides well-studied and weakly interacting rare-gas clusters as the environment. Experiments are conducted with solid rare-gas clusters of argon and neon doped with free-base phthalocyanine (H_2Pc) and interrogated with action-based two-dimensional electronic spectroscopy. The high spectro-temporal resolution of this technique allows us to resolve subtle changes in binding configurations with femtosecond precision. We report an anomalous diffusion behavior of H_2Pc in both of the dopant-host nanosystems on a picosecond timescale. Molecular dynamics simulations confirm these findings and further reveal that movement of H_2Pc is confined to rotations on a single facet of the icosahedral host cluster.

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

Time: Friday 11:00–13:00

Location: HS XV

Invited Talk

MO 29.1 Fri 11:00 HS XV

N_2 activation by transition metal clusters — MAX LUCZAK, CHRISTOPHER WIEHN, DANIELA FRIES, NIELS WOLFGRAMM, CHRISTOPH VAN WÜLLEN, and ●GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie, RPTU Kaiserslautern-Landau

Size selected transition metal (TM) cluster cations and anions attach N_2 molecules under single collision cryo conditions, and they may or may not subsequently activate the adsorbates. Cryo kinetics and infrared spectra reveal details that serve to model the activation pathways by DFT calculations [1,2,3]. It shows that there is a quite general multi-step-pathway. Energetics vary by the particular TM but corresponding intermediates along the pathways seem quite similar amongst the investigated TMs. We aim to put these findings to the stage and present our current understanding for further discussions.

[1] Phys. Chem. Chem. Phys. **23**, 11345 (2021); DOI: 10.1039/D0CP06208A

[2] J. Chem. Phys. **159**, 164306 (2023); DOI: 10.1063/5.0157218

[3] J. Chem. Phys. **159**, 164303 (2023); DOI: 10.1063/5.0157217

MO 29.2 Fri 11:30 HS XV

Dynamics of CO_2 activation by transition metal ions — ●MARCEL META, MAXIMILIAN E. HUBER, MARTIN WEDELE, and MARCEL META — RPTU Kaiserslautern-Landau und Forschungszentrum OPTIMAS, Fachbereich Chemie, Kaiserslautern, Germany

Here, we present a joint experimental and theoretical study of the dynamics of ion-molecule reactions. We focus on the oxygen atom transfer (OAT) reaction between transition metal ions and carbon dioxide $M^+ + CO_2 \rightarrow MO^+ + CO$ ($M^+=Ta^+, Nb^+, Zr^+$) [1,2]. Indirect dynamics were observed for all reactions, despite the fact that the thermal rates are close to the collision rate and the reaction is exothermic

in all cases. The investigated reactions have a multi-state character and require an inter-system crossing (ISC) for their occurrence. These findings indicate the presence of a bottleneck along the reaction. The nature of the bottleneck (submerged transition state versus ISC) was investigated in a collaborative effort.

In order to achieve this, angle and energy differential cross-sections were measured using 3D velocity map imaging at different collision energies. Thermal rate constants were obtained using selected ion flow tube (SIFT). These experimental findings were supplemented by high-level theory and trajectory simulations [3]. In addition, this approach allows us to make precise assertions regarding the distribution of energy. [1] M. E. Huber et al. 8670, 26, Phys. Chem. Chem. Phys. (2024). [2] M. Meta et al., 5524, 14, J. Phys. Chem. Lett (2023). [3] Y. Liu et al. J. Am Chem. Soc., 14182, 146 (2024).

MO 29.3 Fri 11:45 HS XV

Insights into Facile Methane Activation by Transition Metal Ions via Intersystem Crossing — 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 for processes like single atom catalysis can be the study of isolated transition metal ion molecule reactions in the gas phase [1,2]. Here, we present a study of kinetics and dynamics on the activation of methane (CH_4) by transition metal cations $M^+ + CH_4 \rightarrow MCH_2^+ + H_2$. The nominally spin-forbidden reaction requires intersystem crossing (ISC) to proceed. 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 carbene formation in the reaction with tantalum

Ta⁺ [3]. The reaction shows dominantly indirect dynamics which is associated to the formation of a long-lived intermediate complex. Experiments for Ta⁺ are furthermore complemented by the reaction of CH₄ with zirconium Zr⁺. In addition recent preliminary theoretical studies confirmed our observations regarding the reaction with Ta⁺ and also 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

MO 29.4 Fri 12:00 HS XV

Relaxation of solvated electrons in the presence of ammonia orbital vacancies — ●AARON NGAI¹, DOMINIQUE DOMINIQUE², LUKAS BRUDER¹, WENTAO CHEN¹, ALEKSANDR DEMIANENKO¹, MICHELE DI FRAIA³, KATRIN DULITZ⁴, IOANNIS MAKOS¹, EVANGELOS MILIORDOS⁵, SITANATH MONDAL¹, OKSANA PLEKAN⁶, SOORAJ RAJENDRAN¹, FABIAN RICHTER¹, NIKLAS SCHEEL⁷, BRENDAN WOUTERLOOD¹, BRUCE YODER², CARLO CALLEGARI⁶, MARCEL MUDRICH⁷, GIUSEPPE SANSONE¹, RUTH SIGNORELL², FRANK STIENKEMEIER¹, and SEBASTIAN HARTWEG¹ — ¹Institute of Physics, University of Freiburg, Germany — ²Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland — ³CNR - Istituto Officina dei Materiali (IOM), S.S. 14, Km 163.5, 34149 Trieste, Italy — ⁴Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria — ⁵Department of Chemistry and Biochemistry, Auburn University, AL, US — ⁶Elettra - Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy — ⁷Department of Physics and Astronomy, Aarhus University, Denmark

Solvated electrons in alkali-metal ammonia solutions are fascinating species that motivate fundamental and applied studies from different fields of research. In synthetic chemistry, these solvated electrons are used as powerful reducing agents in challenging reduction reactions [1]. From a physical perspective, they exhibit peculiar concentration-dependent properties and processes, such as the spin-pairing of solvated electrons and the phase transition to a metallic state at high concentrations [2]. Recently, a photoionization study of sodium-doped ammonia clusters, revealed the production of low-energy electrons from electron-transfer mediated decay of solvated electron pairs formed by optical excitation [3]. Motivated by the observation of this optically-triggered autoionization process, we performed a time-resolved photoelectron spectroscopy study of sodium-doped ammonia clusters with extreme ultraviolet radiation at the free-electron laser FERMI. I will present preliminary results of this study, which reveals the dynamics of solvated electrons in the vicinity of ammonia valence shell vacancies and the effects of excitations induced by ultraviolet light in these fascinating cluster systems.

[1] Birch, A.J. *J. Chem. Soc.*, **0**, 430-436 (1944)
[2] Zureck, E. *et al. Angew. Chem. Int. Ed.* **48**, 44 (2009)
[3] Hartweg, S. *et al. Science* **380**, 6650 (2023)

MO 29.5 Fri 12:15 HS XV

Droplet shape and quantum vortices visualized by the spectral shape of the electronic band origin of phthalocyanine doped into superfluid helium nanodroplets — ●RUPERT JAGODE and ALKWIN SLENCZKA — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93053 Regensburg

With the help of X-ray diffraction, the global shape of superfluid helium droplets could be imaged [1]. In addition, the inner structure, which may consist of quantum vortices - a specific form of angular momentum in quantum liquids - also became visible. These findings provide a consistent interpretation for the evolution of the spectral

shape at the electronic band origin of phthalocyanine with increasing droplet size. Both the droplet shape and the presence of quantum vortices should have an effect on the solvent shift of the electronic transitions of the dopant molecule. New lineshape studies were carried out with systematic variation of the effective droplet sizes and optical anisotropy studies. From these new data, some of the still open questions regarding a reversal of the solvent shift [2] as well as the imperfect reproducibility of the observed signal splitting [2] could be clarified. Obviously, electronic spectroscopy complements the observations from X-ray diffraction on droplet shapes and the presence of quantum vortices for a range of smaller droplet sizes, which are relevant as host systems in molecular spectroscopy.

[1] B. Langbehn et al., *Phys.Rev.Lett.* 121, 255301 (2018), A. Ulmer et al., *Phys.Rev.Lett.* 131, 076022 (2023). [2] S. Fuchs et al., *J.Chem.Phys.* 148, 144301 (2018).

MO 29.6 Fri 12:30 HS XV

Broadband Femtosecond Transient Absorption Microscopy — ●MAGNUS FRANK, CHRIS REHHAGEN, and STEFAN LOCHBRUNNER — Institute for Physics and Department of Life, Light and Matter, University of Rostock, 18051 Rostock, Germany

Organic crystalline micro- and nanostructures have become of great interest in the field of semiconductors and optoelectronics. In these applications the exciton dynamics play an important role and can determine the suitability of a certain structure. Femtosecond pump probe spectroscopy is the standard method for characterising exciton dynamics but its adoption for use on organic micro- and nanostructures is not without challenge. The main problem is increasing the spatial resolution to a level that a specific structure can be studied while maintaining a high signal to noise ratio. Additionally, tightly focussing spectrally broad light represents another challenge as chromatically compensated optics cannot be used with fs laser pulses. It is for these reasons that typically only single colour experiments are conducted.

In this work we present a transient absorption microscope that is capable of resolving singular nanostructures. We are able to reach a spatial resolution lower than 1 μm and a sub-100 fs time resolution while managing to cover nearly the whole visible spectrum as well as parts of the NIR.

MO 29.7 Fri 12:45 HS XV

Time-resolved UV-vis Spectroelectrochemistry — ●NINA BRAUER¹, RAMISHA RABEYA¹, ROBERT FRANCKE², and STEFAN LOCHBRUNNER¹ — ¹Institute of Physics, University of Rostock, Germany — ²Leibniz Institute for Catalysis, Rostock, Germany

Homogeneous electrocatalysis based on transition metal complexes holds great potential for carbon dioxide utilization. In order to develop an efficient catalytic system, detailed knowledge about each step of the complex reaction chain is highly desirable. Therefore, the identification of short-lived intermediates and the determination of their life-times is of crucial importance here.

Spectroelectrochemistry has proven to be a powerful experimental approach to determine the reaction dynamics during electrocatalytic processes. In this work, a time-resolved UV-vis spectroelectrochemistry setup is developed using laser pulses to achieve a time resolution of microseconds. In contrast to previous work, this enables precise detection of catalytic reaction rates down to the diffusion limit. In the experiment, a femtosecond supercontinuum is focused closely to the working electrode surface inside a custom electrochemical cell based on a quartz glass cuvette. Upon applying a potential step to the electrodes, the induced absorption change inside the diffusion layer is measured as a function of time.

MO 30: Molecular Spectroscopy and Theoretical Approaches

Time: Friday 14:30–16:15

Location: HS XVI

MO 30.1 Fri 14:30 HS XVI

High-resolution rovibrational spectroscopy of H₅⁺ — ●SAMUEL MARLTON, PHILIPP SCHMID, THOMAS SALOMON, JANOS SARKA, DIVITA GUPTA, OSKAR ASVANY, and STEPHAN SCHLEMMER — University of Cologne, Cologne, Germany

H₅⁺ is an extremely floppy molecular ion that is so complex that it pushes the limits of foundational concepts in spectroscopy and molec-

ular physics such as molecular structure, normal modes of vibration, typical group theoretical treatments, and the separation of vibrational and rotational degrees of freedom. Using leak-out spectroscopy (LOS) it is finally possible to measure infrared transitions of H₅⁺ with high resolution.[1] In this experiment, H₅⁺ ions are stored in a cryogenic (20 K) 22-pole ion trap and irradiated with an infrared laser. Photoexcited ions collide with neutral He gas atoms to transfer the vibrational internal energy of the ion into kinetic energy, giving the ion sufficient

kinetic energy to leak out of the trap and be detected. The LOS spectrum is constructed by measuring the leak-out ion yield as a function of laser frequency. We employ LOS to measure the H_5^+ vibrational band centred at 940 cm^{-1} (a combination band exciting the central proton hop and outer hydrogen separation), which is a promising step to understanding extremely floppy molecules.

[1] Schmid *et al.*, 2022, *J. Phys. Chem. A.*, 126(43), pp.8111-8117.

MO 30.2 Fri 14:45 HS XVI

Experimental symmetry assignments of protonated methane rovibrational levels — ●SAMUEL MARLTON, PHILIPP SCHMID, OSKAR ASVANY, and STEPHAN SCHLEMMER — University of Cologne, Cologne, Germany

Protonated methane (CH_5^+) does not consist of one proton and four hydrogen atoms but all five protons are equivalent, all entertaining bonds with the central carbon atom. This makes the molecule floppy with an irregular rovibrational spectrum, which remains unassigned. [1,2] The nuclear spins of the five protons combine to a total nuclear spin of $I = 1/2, 3/2$ or $5/2$, which—due to the Pauli exclusion principle—combine with ro-vibrational states of corresponding symmetry $A_2 \hat{=} I = 5/2$, $G_2 \hat{=} I = 3/2$, and $H_2 \hat{=} I = 1/2$ with abundance ratios of 6:4:2. Using leak-out spectroscopy (LOS), [3] we provide direct experimental symmetry assignments by measuring these abundance ratios. In our experiment, CH_5^+ ions stored in a cryogenic ion trap are irradiated with an infrared laser. Photoexcited ions collide with neutral gas atoms (Ne) to eventually transfer vibrational energy into kinetic energy, giving the ion sufficient kinetic energy to leak out of the trap. We assign symmetry labels to transitions by measuring the fraction ($2/12, 4/12$, or $6/12$) of CH_5^+ ions that leak-out of the trap when each transition is resonantly excited. This approach will help construct a ground state term diagram. [1] White *et al.*, 1999, *Science*, [2] Asvany *et al.*, 2015, *Science*, [3] Schmid *et al.*, 2022, *J. Phys. Chem. A*.

MO 30.3 Fri 15:00 HS XVI

Spatially resolved spectroscopy of Rydberg states in nitric oxide — ●YANNICK SCHELLANDER¹, FABIAN MUNKES², ALEXANDER TRACHTMANN², FLORIAN ANSCHUTZ², ETTORE EDER², HANNA LIPPMANN², MERIEM MAVLUTOVA², MARIUS WINTER¹, ROBERT LÖW², PATRICK SCHALBERGER¹, TILMANN PFAU², HARALD KÜBLER², and NORBERT FRUEHAUF¹ — ¹Institute for Large Area, University of Stuttgart, Stuttgart, Germany — ²5th Institute of Physics, University of Stuttgart, Germany

High-resolution continuous-wave (cw) laser spectroscopy of nitric oxide (NO) molecules has been performed to study the energy-level structure. Special focus is on effects of electric fields on high Rydberg states. The photo-excitation is based on a resonance enhanced three-color three-photon excitation scheme. In contrast to theory, the measurements show states with no frequency shift. The reason for this effect is most likely an inhomogeneous electric field distribution. This is caused by field attenuations near the cell walls resulting from charge carrier accumulations on these. Therefore, charge carriers generated near the cell walls experience a much lower electric field than expected. To further investigate the charge carrier effects and prove the given explanation, spatially resolved measurements of the ionization currents are performed. These kinds of measurements are enabled by an electrode / transimpedance amplifier array based on thin-film technology. Other thinkable applications of such a sensor array could be the determination of the dynamic density distribution by turbulent gas flow or in resonance-enhanced multiphoton ionization experiments.

MO 30.4 Fri 15:15 HS XVI

Recent achievements and future prospects in precision spectroscopy of tritium-substituted molecules — ●VALENTIN HERMANN — Tritiumlabor Karlsruhe, Karlsruhe Institute for Technology, Karlsruhe, Germany

Precision spectroscopy of tritium-substituted molecules provides essential data for refining molecular energy models and supports applications in fusion research, where monitoring tritium-containing species is crucial. Recent advancements include high-resolution FTIR spectroscopy of tritiated water isotopologues (HTO, DTO, T₂O), revealing over 4500 new absorption lines with accuracies up to $5.6 \times 10^{-5}\text{ cm}^{-1}$. NICE-OHMS (Noise-Immune Cavity-Enhanced Optical Heterodyne Molecular Spectroscopy) has also been applied to HT, achiev-

ing unprecedented spectral accuracy of 21 kHz.

Future projects aim to expand high-accuracy measurements to additional tritium-substituted species and to systematically improve line intensities for enhanced spectroscopic databases. The planned investigation of tritiated methane will support fusion research by enabling more accurate detection and monitoring of tritiated hydrocarbons, which are critical for fuel cycle control.

MO 30.5 Fri 15:30 HS XVI

The connection between the Exact Factorization and the Born-Huang representation of the molecular wave function — ●PETER SCHÜRGER¹, YORICK LASSMANN², FEDERICA AGOSTINI¹, and BASILE CURCHOD² — ¹Institut de Chimie Physique, University Paris-Saclay — ²Centre for Computational Chemistry, School of Chemistry, University of Bristol

In recent years, the exact factorization (EF) formalism sparked a lot of interest in the non-adiabatic dynamics community and led to the development of various new promising methods for non-adiabatic molecular dynamics simulations [see e.g. PCCP, 26, 26693-26718 (2024)]. In EF, the molecular wave function is written as a product of a time-dependent conditional and time-dependent marginal amplitude. The EF is usually presented as “qualitatively” different in its formalism, compared to the more traditional Born-Huang (BH) representation, i.e. the adiabatic representation of the molecular wave function [JPC A, 126, 1263-1282 (2022)]. Here, I will present a new perspective on the foundations of EF [ChemRxiv (2024)], that does not rely on a probabilistic interpretation and that strengthens the connection between EF and BH. Specifically, EF is a basis set that can be derived from BH and the adiabatic basis by introducing a time-dependent unitary transformation. Features of the EF, like the partial normalization condition and the gauge freedom, arise naturally in our formalism. Furthermore, equations of motion can be derived in this EF basis. I will conclude by presenting some applications of EF to simulate the ultrafast dynamics of fulvene and 4-(dimethylamino)benzotrile (DMABN).

MO 30.6 Fri 15:45 HS XVI

A Hierarchical Approach to Quantum Many-Body Systems in Structured Environments — KAI MÜLLER¹, KIMMO LUOMA², and ●CHRISTIAN SCHÄFER³ — ¹Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — ²Department of Physics and Astronomy, University of Turku, 20014 Turku, Finland — ³Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Open quantum systems featuring non-Markovian dynamics are routinely solved using techniques such as the Hierarchical Equations of Motion (HEOM) but their usage of the system density-matrix renders them intractable for many-body systems. Here, we combine the HEOM with the BBGKY hierarchy to reach a consistent and rigorous description of open many-body systems and their quantum dynamics. [Kai Müller, Kimmo Luoma, and Christian Schäfer, arXiv:2405.05093.] We demonstrate first the strength and limitations of this stacked hierarchy for superradiant emission and spin-squeezing of established quantum optical models before presenting its full potential for quantum many-body systems. In particular, we explicitly simulate the impact of charge noise on the dynamic of the Fermi-Hubbard model subject to a structured bath comprising cavity and vibro-phononic environment. Lastly, we discuss few-emitter lasing to further elaborate the flexibility of the stacked hierarchy. Our work establishes an accessible, yet rigorous, route between condensed matter and quantum optics, fostering the growth of a new domain at their interface.

MO 30.7 Fri 16:00 HS XVI

Calculating excitonic interactions using transition currents with application to PTCDA — ●GRACE HSIAO-HAN CHUANG and ALEXANDER EISEFELD — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str 38, Dresden

We calculate the excitonic interaction of the PTCDA dimer without overlapping molecular wavefunctions, focusing on transition charge and current density. These quantities are derived from post-processing the numerical wavefunction using electronic structure theory. Additionally, we present a homemade algorithm designed to efficiently and cost-effectively capture these two quantities. To validate the dipole approximation, we also compute accurate numerical values for a typical arrangement of PTCDA on a monolayer.