

Molecular Physics Division Fachverband Molekülphysik (MO)

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Overview of Invited Talks and Sessions

(Lecture halls H1, H2, and H3; Poster P)

Invited Talks

MO 1.1	Mon	10:45–11:15	H2	Long-range interactions between polar molecules and Rydberg atoms — •MARTIN ZEPPENFELD
MO 3.1	Tue	10:45–11:15	H3	Photoelectron circular dichroism in the light of resonance enhanced multi-photon ionization — •THOMAS BAUMERT

Invited talks of the joint symposium Trends in atom interferometry (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Mon	14:00–14:30	Audimax	Atom interferometry and its applications for gravity sensing — •FRANCK PEREIRA DOS SANTOS, LUC ABSIL, YANN BALLAND, SÉBASTIEN MERLET, MAXIME PESCHE, RAPHAËL PICCON, SUMIT SARKAR
SYAI 1.2	Mon	14:30–15:00	Audimax	Atom interferometry for advanced geodesy and gravitational wave observation — •PHILIPPE BOUYER
SYAI 1.3	Mon	15:00–15:30	Audimax	3D printing methods for portable quantum technologies — •LUCIA HACKERMÜLLER
SYAI 1.4	Mon	15:30–16:00	Audimax	Fundamental physics with atom interferometry — •PAUL HAMILTON

Invited talks of the joint symposium SAMOP Dissertation Prize 2021 (SYAD)

See SYAD for the full program of the symposium.

SYAD 1.1	Tue	10:45–11:15	Audimax	Attosecond-fast electron dynamics in graphene and graphene-based interfaces — •CHRISTIAN HEIDE
SYAD 1.2	Tue	11:15–11:45	Audimax	About the interference of many particles — •CHRISTOPH DITTEL
SYAD 1.3	Tue	11:45–12:15	Audimax	Supersolid Arrays of Dipolar Quantum Droplets — •FABIAN BÖTTCHER
SYAD 1.4	Tue	12:15–12:45	Audimax	Quantum Logic Spectroscopy of Highly Charged Ions — •PETER MICKE

Invited talks of the joint symposium Chirality meets ultrafast (SYCU)

See SYCU for the full program of the symposium.

SYCU 1.1	Tue	14:00–14:30	Audimax	Overview of the temporal dependencies of Photoelectron Circular Dichroism — •VALERIE BLANCHET
SYCU 1.2	Tue	14:30–14:45	Audimax	Ultrafast, all-optical, and highly enantio-sensitive imaging of molecular chirality — •DAVID AYUSO
SYCU 1.3	Tue	14:45–15:00	Audimax	Hyperfine interactions in rotational chiral states — •ANDREY YACHMENEV

SYCU 1.4	Tue	15:00–15:30	Audimax	Chiral molecules in an optical centrifuge — ●VALERY MILNER, ALEXANDER MILNER, ILIA TUTUNNIKOV, ILYA AVERBUKH
SYCU 1.5	Tue	15:30–16:00	Audimax	Enantiomer-selective controllability of asymmetric top molecules — ●MONIKA LEIBSCHER

Invited talks of the joint symposium Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:15	Audimax	Frequency comb spectroscopy and interferometry — ●NATHALIE PICQUÉ
SYAW 1.2	Wed	14:15–15:00	Audimax	Capitalizing on Schrödinger — ●WOLFGANG P. SCHLEICH
SYAW 1.3	Wed	15:00–15:45	Audimax	Quantum information processing with macroscopic objects — ●EUGENE POLZIK

Invited talks of the joint symposium Hot topics in cold molecules: From laser cooling to quantum resonances (SYCM)

See SYCM for the full program of the symposium.

SYCM 1.1	Fri	14:00–14:30	Audimax	Collisions between laser-cooled molecules and atoms — ●MICHAEL TARBUTT
SYCM 1.2	Fri	14:30–15:00	Audimax	Trapped Laser-cooled Molecules for Quantum Simulation, Particle Physics, and Collisions — ●JOHN DOYLE
SYCM 1.3	Fri	15:00–15:30	Audimax	Quantum-non-demolition state detection and spectroscopy of single cold molecular ions in traps — ●STEFAN WILLITSCH
SYCM 1.4	Fri	15:30–16:00	Audimax	Quantum state tomography of Feshbach resonances in molecular ion collisions via electron-ion coincidence spectroscopy — ●EDVARDAS NAREVICIUS

Sessions

MO 1.1–1.5	Mon	10:45–12:15	H2	Electronic
MO 2.1–2.6	Mon	14:00–15:30	H2	Cluster & Complexes
MO 3.1–3.8	Tue	10:45–13:00	H3	Chirality
MO 4	Wed	13:00–13:30	MVMO	Annual General Meeting
MO 5.1–5.6	Thu	10:45–12:15	H2	Miscellaneous
MO 6.1–6.6	Thu	14:00–15:30	H2	Ultrafast
MO 7.1–7.24	Thu	17:30–19:30	P	Poster 1
MO 8.1–8.8	Fri	10:45–12:45	H1	Cold Molecules
MO 9.1–9.17	Fri	17:30–19:30	P	Poster 2

Annual General Meeting of the Molecular Physics Division

Wednesday 13:30–14:00 MVMO

MO 1: Electronic

Time: Monday 10:45–12:15

Location: H2

Invited Talk

MO 1.1 Mon 10:45 H2

Long-range interactions between polar molecules and Rydberg atoms — ●MARTIN ZEPPENFELD — MPI für Quantenoptik, Hans-Kopfermann Str. 1, 85748 Garching

Due to large dipole moments in polar molecules and huge dipole moments in Rydberg atoms, strong interactions between polar molecules and Rydberg atoms persist for separations beyond $1\ \mu\text{m}$. This provides exciting opportunities in quantum science, with applications such as cooling of internal or motional molecular degrees of freedom, nondestructive molecule detection, and quantum information processing.

In my talk, I will provide an overview of these opportunities and present my work on realizing such ideas experimentally. In particular, we have investigated Förster resonant energy transfer between molecules and Rydberg atoms at room temperature in the past, observing huge interaction cross sections and electric-field-controlled collisions. Currently we are setting up a new experiment to investigate interactions between cold molecules and Rydberg atoms, providing many new opportunities.

MO 1.2 Mon 11:15 H2

Optical Properties of Gold Cations — ●MARKO FÖRSTEL¹, KAI POLLW¹, TAARNA STUEMUND¹, NIKITA KAVKA², ROLAND MITRIC², and OTTO DOPFER¹ — ¹Technische Universität Berlin, Berlin, Deutschland — ²Universität Würzburg, Würzburg, Deutschland

The scientific interest in gold clusters and nanoparticles is very high, especially due to their manifold catalytic properties. In order to understand these in detail, it is necessary to have precise knowledge of the electronic structure of gold-containing systems. We probe the optical properties of small gold clusters in unprecedented detail using highly sensitive photodissociation spectroscopy and compare our results with various theoretical methods to provide a better understanding of these systems. In this talk we summarize our findings on Au_2^+ [1,2], Au_3^+ and Au_4^+ [3,4] clusters.

[1] Förstel et al., *Angewandte Chemie Int. Ed.* 123 48, 2020[2] Förstel et al., submitted to *Eur. J. Chem.*[3] Förstel et al., *Angewandte Chemie Int. Ed.* 58 11, 2019[4] Förstel et al., *Rev. Sci. Instr.* 88 12, 2017

MO 1.3 Mon 11:30 H2

Exploration of the Optical Properties of Small Cationic Silicon Carbides: The Optical Spectrum of $Si_4C_2^+$ — ●ROBERT G. RADLOFF, MARKO FÖRSTEL, KAI POLLW, TAARNA STUEMUND, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany

It is known that a great number of molecules are present in space. Some of these molecules have already been identified, others remain to be discovered. In the environment of carbon stars like IRC+ 10216, where carbon is more abundant than oxygen, not all carbon is bound into CO and thus a variety of carbon bearing molecules exists in the

outer layers of these stars. We focus our research on silicon carbide aggregates. Observations show that small silicon carbide molecules like SiC, Si₂C, SiC₂, SiC₃ and SiC₄ are present in the circumstellar medium around the IRC+ 10216. Furthermore, its spectrum shows an emission feature around $12\ \mu\text{m}$ that is tentatively attributed to silicon carbide dust grains.

In our study we are aiming to gain insight into the optical and structural properties and the photochemistry of small cationic silicon carbides as well as a better understanding of their role in astrochemistry and their influence on the formation of silicon carbide dust grains. We present the photofragmentation behavior of various cationic silicon carbides and the first optical spectrum of $Si_4C_2^+$ recorded by means of photodissociation spectroscopy in the range of 208-330 nm [1].

[1] M. Förstel et al., *J. Mol. Spectrosc.*, 2021, 377, 111427

MO 1.4 Mon 11:45 H2

Near-infrared spectrum of the first excited state of Au_2^+ — ●KAI MARIO POLLW, MARKO FÖRSTEL, TAARNA STUEMUND, and OTTO DOPFER — Technische Universität Berlin, Berlin, Deutschland

We recently observed and published the optical spectrum of the gold dimer cation which resembles the simple H_2^+ molecule in its electronic configuration.[1] Due to the highly irregular spectral structure, multi-reference methods, spin-orbit coupling and relativistic corrections need to be taken into account to understand the PES of this seemingly simple dimer. By tagging with Ar we are able to investigate the otherwise not accessible 1st excited state in the near-infrared. Surprisingly, this state shows a regular vibronic structure that can be well reproduced by DFT calculations. In this talk we will present our experimental and computational results on the $Au_2^+ - Ar$ system.

[1] Förstel et al., *Angewandte Chemie Int. Ed.* 123 48, 2020

MO 1.5 Mon 12:00 H2

X-ray L-edge absorption spectroscopy on gas phase diatomic iron halide systems beyond the oxidation state — ●MAX FLACH^{1,2}, VICENTE ZAMUDIO-BAYER¹, KONSTANTIN HIRSCH¹, MARTIN TIMM¹, OLESYA ABLYASOVA^{1,2}, MAYARA DA SILVA SANTOS DA SILVA SANTOS^{1,2}, MARKUS KUBIN KUBIN¹, CHRISTINE BÜLOW², BERND VON ISSENDORFF², and TOBIAS LAU^{1,2} — ¹Helmholtz-Zentrum, Berlin, Germany — ²Albert-Ludwigs-Universität, Freiburg, Germany

Transition Metal L-edge spectroscopy is widely used to determine oxidation states of a wide range of samples, hence, an estimate of uncertainty contributions to assigned oxidation states from chemical shifts is of high importance. Here we use gas phase FeX^+ ($X=F, Cl, Br, I$) as a idealized model system to provide high resolution XAS spectra to quantify energy shifts of the Iron L₃-edge and to study changes in electronic structure within the same oxidation state of Fe(II). Along with a change in line shape of the Iron L₃-edge, we observe energy shifts of the intensity distributions median of the spectra along the series. The observed shifts hint towards a charge transfer to and from the halogen to the iron, involving orbitals of different symmetry.

MO 2: Cluster & Complexes

Time: Monday 14:00–15:30

Location: H2

MO 2.1 Mon 14:00 H2

$Si_nO_m^+$ - Optical Absorption and Photodissociation Properties — ●TAARNA STUEMUND, MARKO FÖRSTEL, KAI POLLW, ROBERT G. RADLOFF, LARS DAHLÖF, JULIAN VOSS, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Deutschland

The origin as well as evolutionary formation mechanisms of stars and solar systems like our own are still poorly understood. Therefore, it is essential to gain a better understanding of interstellar dust, as it is a major actor in this process. So far, it is known that such dust contains μm -sized silicate particles. On the other hand, the only molecular species that has been found in the interstellar matter (ISM) which could be a direct precursor to silicate dust is SiO [1]. To this end we present both, experimental data and quantum chemical calculations,

that help to understand the dissociation and absorption behavior of possible intermediate silicon-oxide species. The ions under investigation were generated in a laser vaporization source, mass-selected and photodissociated [2]. The resulting absorption spectra are compared to TD-DFT calculations and discussed in an astrophysical context.

[1] R. Wilson et al., 1971, *Astrophys. J.* 167, L97 [2] M. Förstel et al., *Rev. Sci. Instrum.*, 2017, 88, 123110.

MO 2.2 Mon 14:15 H2

Time-resolved photon interactions of size- and charge-state selected polyanionic tin clusters — ●ALEXANDER JANKOWSKI, MORITZ GRUNWALD-DELITZ, and LUTZ SCHWEIKHARD — Institute of Physics, University of Greifswald, Germany

In contrast to many other metals, small tin clusters (Sn_n^- of sizes $n \lesssim 50$) are formed by so-called building blocks of Sn_7 , Sn_{10} [1-3] and, in the case of anionic clusters, Sn_{15} [3]. These cluster sizes $n = 7, 10$ and 15 lead to corresponding fragmentation patterns [4,5] which have been confirmed and further investigated [6,7] at the ClusterTrap setup [8]. These previous findings suggested for dianionic tin clusters fission processes into two monoanionic fragments in analogy to the case of lead clusters [9]. Recently, photodissociation experiments have been performed on size- and charge-state-selected polyanionic tin clusters. By delaying the ejection/analysis of the trapped clusters with respect to the pulsed photoexcitation, time-resolved measurements allow the reconstruction of the decay pathways.

- [1] C. Majumder et al., *Phys. Rev. B* **64**, 233405 (2001)
- [2] H. Li et al., *J. Phys. Chem. C* **116**, 231-236 (2011)
- [3] A. Lechtken et al., *J. Chem. Phys.* **132**, 211102 (2010)
- [4] E. Oger et al., *J. Chem. Phys.* **130**, 124305 (2009)
- [5] A. Wiesel et al., *Phys. Chem. Chem. Phys.* **14**, 234-245 (2012)
- [6] S. König et al., *Eur. Phys. J. D* **72**, 153 (2018)
- [7] M. Wolfram et al., *Eur. Phys. J. D* **74**, 135 (2020)
- [8] F. Martinez et al., *Int. J. Mass Spectrom.* **266**, 365-366 (2014)
- [9] S. König et al., *Phys. Rev. Lett.* **120**, 163001 (2018)

MO 2.3 Mon 14:30 H2

N_2 Cleavage by Tantalum Cluster under Cryo Conditions — •DANIELA V. FRIES, MATTHIAS P. KLEIN, ANNIKA STRASSNER, MAXIMILIAN HUBER, MARC H. PROSENC, and GEREON NIEDNER-SCHATTEBURG — TU Kaiserslautern, Kaiserslautern, Deutschland

As motivated by prior room temperature studies on Ta_n^+ [1] we investigate larger Ta_n^+ clusters ($4 < n < 7$) and their N_2 adsorption and activation abilities by adsorption kinetics and infrared spectroscopy under cryo conditions compared with DFT calculations.

The model system Ta_4^+ appears to be of particular interest with regard to cryo N_2 activation. Experimental results reveal peculiar details for the first and second adsorption kinetics, and the infrared signatures show no NN stretching bands in $[\text{Ta}_4(\text{N}_2)_1]^+$ and $[\text{Ta}_4(\text{N}_2)_2]^+$. This is consistent with cleavage of the first two adsorbed dinitrogen molecules and we unravel a multistep above edge across surface (AEAS) mechanism for the cleavage of first and second N_2 adsorbates. Cleavage of the third N_2 ligand is kinetically hindered. We recognize that substoichiometric N_2 exposure allows for spontaneous activation by Ta_4^+ , while higher N_2 exposure causes self poisoning.[2]

- [1] Proc. Natl. Acad. of Sci. USA, 2018, 115, 11680-11687.
- [2] Phys. Chem. Chem. Phys., 2021, 23, 11345-11354.

MO 2.4 Mon 14:45 H2

Combined IR/UV spectroscopic and quantum chemical studies on chromone/methanol aggregates — •PATRICK HORST STREBERT, POL BODEN, MARCEL META, CHRISTOPH RIEHN, and MARKUS GERHARDS — Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern, Research Center Optimas and Technical University Kaiserslautern

Dispersion forces have often been underestimated in the description of intra- and intermolecular interactions. Within aggregates, the balance between dispersion interactions and electrostatic forces can be the deciding factor for the preference of a certain binding motif and can be difficult to model with current theoretical methods. Systematic probing of dispersion interactions in aggregates with two or more possible binding motifs enables better understanding and description of these phenomena.

In this work, complexes of chromone with methanol were investigated by IR/UV laser spectroscopy in a molecular beam experiment.

The experimental results are compared to theoretical predictions obtained from (TD)DFT-, DLPNO-CCSD(T)- and SAPT-calculations, including transition state calculations with respect to different isomers. The chromone molecule provides two binding sites at the carbonyl oxygen enabling us to study the balance of electrostatic and dispersion forces in the electronic ground state (S_0) as well as the electronically excited triplet state (T_1). To the best of our knowledge, we present the first IR investigations of isolated aggregates (gas phase) between an alcohol and another organic molecule in a triplet state.

MO 2.5 Mon 15:00 H2

Multi-spectroscopic investigations of NIR emissive Cr(0), Mo(0) and W(0) complexes — •PIT BODEN¹, PATRICK DI MARTINO-FUMO¹, SOPHIE STEIGER¹, TOBIAS BENS², BIPRAJIT SARKAR², GEREON NIEDNER-SCHATTEBURG¹, and MARKUS GERHARDS¹ — ¹TU Kaiserslautern, Fachbereich Chemie and Research Center Optimas, Kaiserslautern — ²University of Stuttgart, Institute of Inorganic Coordination Chemistry, Stuttgart

In this contribution^[1] a multi-spectroscopic approach is applied for the photophysical and structural characterization of NIR emissive Cr(0), Mo(0) and W(0) carbonyl complexes containing a pyridyl-mesoionic carbene ligand. The idea is to replace luminophores based on rare-earth metals like e.g. iridium and lanthanides by more abundant elements.

Luminescence spectroscopy at variable temperature on solid samples revealed a dual emission ($\lambda_{\text{VIS}} = 666 - 700 \text{ nm}$, $\lambda_{\text{NIR}} = 918 - 950 \text{ nm}$, depending on the metal center) at room temperature and an increase of the quantum yields upon cooling to 5 K. The luminescence bands are assigned to phosphorescence according to the lifetimes obtained by time-resolved luminescence and step-scan FTIR spectroscopy. Furthermore, the step-scan FTIR analysis revealed small but significant variations of CO bond lengths in the excited state, in combination with density functional theory calculations. An excited triplet state of metal-to-ligand charge transfer character was attributed to the visible emission.

- [1] P. Boden et al., *Chem. Eur. J.* **2021**, accepted.

MO 2.6 Mon 15:15 H2

Influence of metal and halide substitution on the photophysics of dinuclear copper(I) and silver(I) complexes — •SOPHIE STEIGER¹, PIT BODEN¹, FLORIAN REHAK², JASMIN BUSCH³, STEFAN BRÄSE³, WIM KLOPPER², GEREON NIEDNER-SCHATTEBURG¹, and MARKUS GERHARDS¹ — ¹TUK, FB Chemie and Research Center Optimas, Kaiserslautern — ²KIT, Institut für Physikalische Chemie, Karlsruhe — ³KIT, Institut für Organische Chemie, Karlsruhe

This contribution presents the investigation of dinuclear copper and silver complexes with a butterfly shaped M_2X_2 core ($\text{M} = \text{Cu}, \text{Ag}$; $\text{X} = \text{Cl}, \text{Br}$). By systematically exchanging the metal and halide centers, the influence of the metals and halides on the photophysical properties is analyzed by using UV/VIS absorbance and (time-resolved) luminescence spectroscopy. Structural information about the excited states were obtained by time-resolved step-scan FTIR spectroscopy combined with quantum chemical TDDFT calculations. The presented spectroscopic experiments are performed at different temperatures (from 290 K to 5 K) to analyze thermally activated or suppressed photophysical processes (e.g. thermally activated delayed fluorescence, TADF). For the presented complexes, the metal exchange has a huge impact on the radiative deactivation channel and the structure of the excited states, whereas the halide exchange has a much smaller influence. Both copper complexes show a red-shift of the emission band from TADF to phosphorescence while cooling down while a strong increase of the emission intensity without relevant spectral shift is observed for the silver complexes.

MO 3: Chirality

Time: Tuesday 10:45–13:00

Location: H3

Invited Talk

MO 3.1 Tue 10:45 H3

Photoelectron circular dichroism in the light of resonance enhanced multi-photon ionization — •THOMAS BAUMERT — Universität Kassel / D-34132 Kassel

Exploiting an electric dipole effect in ionization [1], photoelectron circular dichroism (PECD) is a highly sensitive enantiospecific spec-

troscopy for studying chiral molecules in the gas phase using either single-photon ionization [2] or multi-photon ionization [3]. In the latter case resonance enhanced multi-photon ionization (REMPI) gives access to neutral electronic excited states. The PECD sensitivity opens the door to study control of the coupled electron and nuclear motion in enantiomers. A prerequisite is a detailed understanding of PECD in REMPI schemes. In this contribution I will report on our recent

experiments devoted to unravel different aspects of this effect on the fenchone prototype by addressing the range from impulsive excitation on the femtosecond time scale to highly vibrational state selective excitation with the help of high resolution nanosecond laser techniques. The reflection of the number of absorbed photons in the PECD will be discussed as well as subcycle effects in bichromatic fields.

- [1] B. Ritchie, *Phys. Rev. A* 1976, 13, 1411-1415.
 [2] N. Bowering, T. Lischke, B. Schmidtke, N. Müller, T. Khalil, U. Heinzmann, *Phys. Rev. Lett.* 2001, 86, 1187-1190.
 [3] C. Lux, M. Wollenhaupt, T. Bolze, Q. Liang, J. Köhler, C. Sarpe, T. Baumert, *Angew. Chem. Int. Ed.* 2012, 51, 5001-5005.

MO 3.2 Tue 11:15 H3

Chiral control of spin-crossover dynamics in Fe(II) complexes — ●MALTE OPPERMAN¹, FRANCESCO ZINNA^{2,3}, JÉRÔME LACOUR³, and MAJED CHERGUI¹ — ¹École Polytechnique Fédérale de Lausanne, Switzerland — ²Università di Pisa, Italy — ³Université de Genève, Switzerland

Fe(II)-based spin-crossover (SCO) complexes hold tremendous promise as multifunctional switches in molecular devices. However, real-world technological applications require the excited spin-states to be kinetically stable - a feature that has thus far only been achieved at cryogenic temperatures. In this respect, Fe(II)(bpy)₃ has emerged as a prototypical model system in support of a single reaction coordinate model, where the back-SCO is governed by a symmetric stretching mode of the metal-ligand bonds, preserving the chiral configuration of the complex. Through a newly developed ultrafast circular dichroism technique combined with transient absorption and anisotropy measurements on Fe(II)(4,4'-dimethyl-2,2'-bpy)₃ in solution, associated for stereocontrol with enantiopure TRISPHAT anions, we now show that this picture is incomplete: the decay of the photoexcited high-spin (HS) state is accompanied by ultrafast changes of its optical activity, reflecting the coupling to a symmetry-breaking torsional twisting mode. Moreover, we show that the ion-pairing interaction with the enantiopure anions suppresses the vibrational population of this mode, thereby achieving a four-fold extension of the HS lifetime. This novel strategy may thus significantly improve the kinetic stability of Fe(II)-based magnetic switches at room temperature.

MO 3.3 Tue 11:30 H3

Coincident measurement of photoion circular dichroism and photoelectron circular dichroism of Propylene Oxide and 1-Phenyl-Ethylamine — ●CARL STEFAN LEHMANN and KARL-MICHAEL WEITZEL — Philipps-Universität Marburg, Chemistry Department

Two methods for chirality analysis based on circular dichroism in laser ionization have gathered attention in recent years: photo-ion circular dichroism (PICD) and photo-electron circular dichroism (PECD). In PICD, a difference in total ion yields upon multiphoton ionization with circular polarized light is measured [1,2], whereas in PECD, the circular dichroism is observed in the angular distribution of the photoelectrons [3,4]. However, PICD and PECD rely on different selection rules and until recently no experiments have been reported in which both effects have been observed simultaneously. Here, we report the first coincident measurement of the PICD and PECD effects. A home-built photoion photoelectron coincidence spectrometer has been used to measure both the PICD and the PECD effects simultaneously employing a high repetition fs-laser system. As examples fs-PICD-PECD coincidence results are presented for parent and fragment ions of R- and S-methyloxirane [5] and R- and S- 1-Phenyl-Ethylamine [6].

- [1] U. Boesl, A. Bornschlegel, *ChemPhysChem*, 2006, 7, 2085-2087.
 [2] P. Horsch, et al., *PCCP*, 2011, 13, 2378-2386. [3] C.S. Lehmann, et al., *J. Chem. Phys.*, 2013, 139, 234307. [4] C. Lux, et al., *Angew. Chem Int Ed.*, 2012, 51, 5001*5005. [5] C.S. Lehmann, K.-M. Weitzel, *PCCP*, 22, 13707, (2020) [6] C.S. Lehmann, K.-M. Weitzel, to be published

MO 3.4 Tue 11:45 H3

Structuring light's chirality to induce enantio-sensitive light bending — ●ANDRÉS ORDÓÑEZ^{1,2}, DAVID AYUSO^{1,3}, PIERO DECLEVA⁴, MISHA IVANOV^{1,3}, and OLGA SMIRNOVA^{1,5} — ¹Max-Born-Institut, Berlin, Germany — ²ICFO, Barcelona, Spain — ³Imperial College London, London, UK — ⁴Università degli studi di Trieste, Trieste, Italy — ⁵Technische Universität Berlin, Berlin, Germany

We show how to structure light's local chirality, a new type of chirality which is effective within the electric-dipole approximation and is relevant for non-linear light-matter interactions. We introduce and realize

an enantio-sensitive interferometer for efficient chiral recognition without magnetic interactions, which can be seen as an enantio-sensitive version of Young's double slit experiment. We show that if the distribution of light's handedness breaks left-right symmetry, the interference of chiral and achiral parts of the molecular response leads to unidirectional bending of the emitted light, in opposite directions in media of opposite handedness. Our work introduces the concepts of polarization of chirality and chirality-polarized light, exposes the immense potential of sculpting light's local chirality, and offers novel opportunities for efficient chiral discrimination and imaging on ultrafast time scales in the highly non-linear regime of light-matter interaction.

MO 3.5 Tue 12:00 H3

Enantioselective Control of Chiral Molecules Induced by Laser and THz Fields with Shaped Polarization — ●ILIA TUTUNNIKOV¹, LONG XU¹, PAUL BRUMER², ALEXANDER A. MILNER³, VALERY MILNER³, ROBERT W. FIELD⁴, KEITH A. NELSON⁴, YEHIAM PRIOR¹, and ILYA SH. AVERBUKH¹ — ¹Weizmann Institute of Science, Rehovot, Israel — ²University of Toronto, Toronto, Canada — ³University of British Columbia, Vancouver, Canada — ⁴Massachusetts Institute of Technology, Cambridge, USA

It has been predicted [1-3] that laser fields with shaped polarization induce transient and persistent enantioselective field-free orientation of chiral molecules. Here, we report the first experimental observation of this phenomenon [4-6] using propylene oxide molecules spun by an optical centrifuge—a laser pulse, whose linear polarization undergoes an accelerated rotation around its propagation direction. In addition, we theoretically demonstrate that a pair of cross-polarized THz pulses, interacting with chiral molecules through their permanent dipole moments, induce a similar enantioselective effect [7]. The demonstrated long-time field-free enantioselective orientation opens new avenues for optical manipulation, discrimination, and, potentially, separation of molecular enantiomers.

- [1] *Phys. Rev. Lett.* **117**, 033001 (2016); [2] *Phys. Rev. Lett.* **120**, 083204 (2018); [3] *J. Phys. Chem. Lett.*, **9**, 1105-1111 (2018); [4] *Phys. Rev. A* **100**, 043406 (2019); [5] *Phys. Rev. Lett.* **122**, 223201 (2019); [6] *Phys. Rev. A* **101**, 021403(R) (2020); [7] *Phys. Rev. Research* **3**, 013249 (2021)

MO 3.6 Tue 12:15 H3

Signatures for chiral enantiomers of a dual p38α MAPK/PDE-4 inhibitor CBS3595 using DFT calculations — ●MADELINE VAN DONGEN¹, FENG WANG¹, ANDREW CLAYTON¹, and ZONGLI XIE² — ¹Swinburne University of Technology, Melbourne, Victoria 3122, Australia — ²CSIRO Manufacturing, Private bag 10, Clayton South, Victoria 3169, Australia

Most biological molecules are naturally present in only one of their chiral forms, hence the binding affinity for a chiral drug can differ for diastereomers and between enantiomers. In clinical environments enantiomers of drugs may have reduced, no, or even deleterious effects. This underscores the need to avoid unknown chiral mixtures and focus on chiral synthesis. Hence, the United States Food and Drug Administration (FDA) issued guidelines and policies in 1992 requiring that absolute stereochemistry be known early in drug development. The less experimental effort spent on unsuccessful compounds, the greater the reduction of time and cost. Instead, a computer based rational approach can justify the selection of a chiral entity. In the present study, we use density functional theory (DFT) to explore measurable properties of chiral CBS3595 (N-{4-[5-(4-Fluorophenyl)-3-methyl-2-methylsulfanyl-3H-imidazol-4-yl]-pyridin-2-yl}-acetamide), a potent dual inhibitor of mitogen activated protein kinase (MAPK) p38α and phosphodiesterase-4 (PDE-4) with promisingly low toxicity, in order to differentiate the enantiomers. Preliminary spectroscopic properties of the enantiomers such as IR, VCD, NMR are presented.

MO 3.7 Tue 12:30 H3

High-Sensitivity and Rapid Measurements of Broadband Optical Activity with Interferometric Fourier-Transform Balanced Detection — ●SOUMEN GHOSH¹, GEORG HERINK², ANTONIO PERRI^{1,3}, FABRIZIO PREDÀ^{1,3}, CRISTIAN MANZONI⁴, DARIO POLLI^{1,3,4}, and GIULIO CERULLO^{1,3,4} — ¹Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy — ²Experimental Physics VIII, University of Bayreuth, D-95447 Bayreuth, Germany — ³NIREOS S.R.L., Via G. Durando 39, 20158 Milano, Italy — ⁴Istituto di Fotonica e Nanotecnologie (IFN) - CNR, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy

We present a novel configuration for high-sensitivity and rapid mea-

surement of broadband CD and ORD spectra spanning the visible and near-infrared. The setup utilizes a linearly polarized light that creates an orthogonally polarized weak chiral free-induction-decay field, along with a phase-locked achiral transmitted signal which serves as the local oscillator for heterodyne amplification. By scanning the delay between the two fields with a birefringent common-path interferometer and recording their interferogram with a balanced detector, broadband CD and ORD spectra are retrieved simultaneously with a Fourier transform. Using an incoherent thermal light source, we achieve state-of-the-art sensitivity for CD and ORD across a broad wavelength range with a measurement time of just a few seconds. The setup allows high-sensitivity measurement of glucose concentration and real-time monitoring of fast asymmetric chemical reactions. The setup can further be extended for broadband transient optical activity measurements.

MO 3.8 Tue 12:45 H3

Molecular Spectroscopy in a Chiral Cavity: Polariton Ring Currents and Circular Dichroism of Mg-porphyrin — ●SHICHAO SUN, BING GU, and SHAUL MUKAMEL — Department of Chemistry and Department of Physics and Astronomy, University of California, Irvine, United States

Time reversal symmetry can be broken by placing a Mg-porphyrin molecule in a chiral optical cavity, thus generating polariton ring currents even with linearly polarized light. These currents induce a circular dichroism signal. Since the electronic state degeneracy in the molecule is lifted by the formation of chiral polaritons, this signal is one order of magnitude stronger than the bare molecule signal induced by circularly polarized light. Controlling photochemical processes by chiral optical cavities is an intriguing future direction.

MO 4: Annual General Meeting

Time: Wednesday 13:00–13:30

Location: MVMO

Annual General Meeting

MO 5: Miscellaneous

Time: Thursday 10:45–12:15

Location: H2

MO 5.1 Thu 10:45 H2

Dissociative recombination of OH⁺ at the Cryogenic Storage Ring — ●ÁBEL KÁLOSI^{1,2}, KLAUS BLAUM², LISA GAMER², MANFRED GRIESER², ROBERT VON HAHN², LEONARD W. ISBERNER^{2,3}, JULIA I. JÄGER², HOLGER KRECKEL², DANIEL PAUL², DANIEL W. SAVIN¹, VIVIANE C. SCHMIDT², ANDREAS WOLF², and OLDŘICH NOVOTNÝ² — ¹Columbia Astrophysics Laboratory, Columbia University, New York, 10027 New York, USA — ²Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — ³I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

The cosmic-ray ionization rate (CRIR) of atomic H is an important parameter for diffuse interstellar cloud models. The protons from hydrogen ionization by cosmic rays initiate subsequent ion-molecule reactions that lead to the gas-phase formation of complex molecules. OH⁺ forms early in this chain of reactions, but it can be destroyed via dissociative recombination (DR) with free electrons. The combination of chemical models and astronomical observations of OH⁺ enables one to quantitatively estimate the CRIR in diffuse interstellar clouds. Such models require rate coefficients that account for the internal excitation of the reactants. We have stored fast OH⁺ ion beams in the cryogenic environment of CSR, where infra-red active diatomic hydrides will relax to their lowest rotational states within minutes of storage. Here, we present merged beams DR experiments for OH⁺ interacting with free electrons produced in a low-energy electron cooler, probing collisions at translational temperatures as low as ~ 10 K.

MO 5.2 Thu 11:00 H2

Electron recombination of rotationally cold CH⁺ molecules — ●DANIEL PAUL^{1,2}, MANFRED GRIESER¹, ROBERT VON HAHN¹, ÁBEL KÁLOSI^{1,2}, CLAUDE KRANTZ¹, HOLGER KRECKEL¹, DAMIAN MÜLL¹, DANIEL W. SAVIN², PATRICK WILHELM¹, ANDREAS WOLF¹, and OLDŘICH NOVOTNÝ¹ — ¹Max-Planck-Institut für Kernphysik, Heidelberg, Germany — ²Columbia Astrophysics Laboratory, Columbia University, New York, NY, USA

Molecular cations in the interstellar medium (ISM) are used to trace the properties of interstellar clouds, out of which stars and planets form. These cations can be destroyed by dissociative recombination (DR) with free electrons. Since calculations of this reaction are challenging, and thus often do not match experimental results, laboratory studies of DR are needed to understand the molecular evolution in space.

We have studied the DR of CH⁺, which is of particular interest for the interpretation of diffuse cloud observations. In the electrostatic cryogenic storage ring CSR, CH⁺ ions in their lowest rovibrational states can be stored for DR experiments under conditions relevant for the diffuse ISM. Using merged ion and electron beams in the CSR electron cooler, low energy (meV) collisions can be studied, corresponding to temperatures on the order of 10 K. We report on experimen-

tal DR rate coefficient results for the CH⁺ rovibrational ground state ($v = 0, J = 0$). In addition, final state branching ratios and angular fragmentation characteristics give a hint for a yet undiscovered dissociative CH state.

MO 5.3 Thu 11:15 H2

Optical Properties of Simple Diamondoid Cations and Their Astrochemical Relevance — ●PARKER B. CRANDALL, ROBERT G. RADLOFF, JAN WEISSFLOG, MARKO FÖRSTEL, and OTTO DOPFER — Technische Universität Berlin, Berlin, Germany

Diamondoids are a class of highly stable, aliphatic cycloalkanes arranged into cage-like structures by sp³ hybridization of the carbon atoms. Similarities between the IR spectra of diamondoids and unidentified infrared emission bands seen in the spectra of young stars with circumstellar disks were found.[1,2] It is also suggested that the radical cations of these molecules, which are predicted to absorb in the IR-UV/VIS range,[3] might be responsible for features in the diffuse interstellar bands. However, the optical spectra of these cations have not been measured experimentally until recently. Here, we present the first optical spectrum of the diamantane radical cation in the gas phase at 5K by trapping in a cryogenic 22-pole ion trap and compare it to the recently reported spectrum of the adamantane radical cation (C₁₀H₁₆⁺).[4] Both spectra reveal broad features in the gas phase, which is attributed to significant lifetime broadening and/or Franck-Condon congestion. Geometric changes due to Jahn-Teller distortion and the astrophysical implications of these ions will also be discussed.

[1] O. Guillois et al., *Astrophys. J.* 1999, 521, L133[2] O. Pirali et al., *Astrophys. J.* 2007, 661, 919[3] M. Steglich et al., *Astrophys. J.* 2011, 729, 91[4] P. B. Crandall et al., 2020, *ApJL*, 900, L20

MO 5.4 Thu 11:30 H2

Penning Electron Spectroscopy of Chiral Camphor Molecules Embedded in Helium Nanodroplets — ●SUBHENDU DE¹, S. MANDAL², SANKET SEN³, L. BEN LTAIEF^{1,4}, RAM GOPAL⁵, R. RICHTER⁶, M. CORENO⁷, S. TURCHINI⁷, D. CATONE⁷, N. ZEMA⁷, M. MUDRICH^{1,4}, V. SHARMA³, and S.R. KRISHNAN¹ — ¹QuCenDiEM group and Dept. of Physics, Indian Institute of Technology Madras, Chennai, India. — ²Indian Institute of Science Education and Research, Pune, India. — ³Indian Institute of Technology Hyderabad, Kandi, India. — ⁴Department of Physics and Astronomy, Aarhus University, Aarhus C. — ⁵Tata Institute of Fundamental Research, Hyderabad, Telangana, India. — ⁶Eletra-Sincrotrone Trieste, Basovizza, Italy — ⁷Istituto di Struttura della Materia - Consiglio Nazionale delle Ricerche (ISM-CNR), Trieste, Italy.

We performed Penning electron spectroscopy of chiral Camphor molecules embedded in cold sub-Kelvin He nanodroplets (~ 0.4 K). We have employed a velocity map imaging (VMI) spectrometer to

measure kinetic energy spectra and angular distributions of photoelectrons in coincidence with photoions detected by the time-of-flight (ToF) technique. When photoexcited at $h\nu = 21.43$ eV, there is a significant transfer of excitation energy from the host atoms to the dopant molecules leading to the Penning ionization [1,2] of the dopant molecules. From these spectra, we discern details of the excited states of fragment ions and photoelectron spectra associated with them.

[1] D. Buchta, et al. 2013 *J. Phys. Chem. A*, 117, 4394.

[2] L. Ben Ltaief et al. 2021 *J Low Temp Phys*, 202, 444-455.

MO 5.5 Thu 11:45 H2

Lifetime of AlF molecules in a dipole trap — ●WEIQI WANG, XIANGYUE LIU, and JESÚS PÉREZ-RÍOS — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

In this work, we construct a six-dimensional potential energy surface (PES) for AlF-AlF collisions based on high-level quantum chemistry method CCSD(T) (coupled-cluster with single and double and perturbative triple excitations) calculations. In addition, we employ machine learning techniques in the interpolative and extrapolative regime to describe the long-range interaction accurately. Finally, we compute the density of states of the complex and analyze its lifetime, and with it, the trapping losses of AlF in a dipole trap.

MO 5.6 Thu 12:00 H2

Combined IR/UV spectroscopic investigations on neutral iso-

lated ion pairs in a molecular beam — ●POL BODEN, MARKUS GERHARDS, and CHRISTOPH RIEHN — TU Kaiserslautern, Fachbereich Chemie and Research Center Optimas, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern

Investigations of neutral isolated ion pairs in the gas phase within the context of Stark effects constitute a still very new field. For these studies, molecular beam experiments combined with IR/UV-laser spectroscopic techniques are an ideal tool, yielding spectra of the free ion pairs which are not affected by any environmental effects, facilitating comparison with quantum chemical predictions. Within this context, the alkali salts (Li-Cs) of para-aminobenzoic acid (PABA) were studied in different electronic states (S_0 and D_0). PABA is a so-called push-pull system, showing rather unique electronic features, with the carboxylate group acting as electron density acceptor, while the amino group donates electron density to the aromatic ring. Hence, for the series of ion pairs, the influence of the reigning electric fields on the electronic behaviour of the distinct compounds can be investigated. More specifically, the often small but considerable IR- and UV-frequency shifts provoked by exchanging the alkali cation (e.g. Li to Na) were followed in detail. A clear correlation between the measured spectral shifts and the distance separating the coordinating alkali cation from the carboxylate anion, depending on the size of the alkali ion (increasing from Li to Cs), is observed and confirmed by quantum chemical calculations (DFT/B3LYP-D3(BJ)/def2-TZVP).

MO 6: Ultrafast

Time: Thursday 14:00–15:30

Location: H2

MO 6.1 Thu 14:00 H2

Ultrafast Spectroscopy of Excited States of Novel Ru and Cu Photosensitizers — ●MIGUEL ANDRE ARGÜELLO CORDERO¹, PIT JEAN BODEN², MARTIN RENTSCHLER⁴, PATRICK DI MARTINO-FUMO², WOLFGANG FREY³, YINGYA YANG⁴, MARKUS GERHARDS², MICHAEL KARNAHL⁴, STEFAN LOCHBRUNNER¹, and STEFANIE TSCHIERLEI⁴ — ¹Institute for Physics, University of Rostock — ²Chemistry Department, TU Kaiserslautern — ³Institute of Organic Chemistry, University of Stuttgart — ⁴Institute of Physical and Theoretical Chemistry, TU Braunschweig

Newly synthesized Ru based photosensitizers with an extended π -system were found to exhibit long lived excited states with lifetimes of 1.7 and 24.7 μ s after optical excitation. The applied biipo ligand coordinates via a phenanthroline moiety, which is extended with a naphthalimide unit. In order to replace the rare noble metal, a Cu based analogue was developed. Nanosecond transient absorption (TA) measurements revealed, that in the Cu complex, non-emissive excited state are populated which exhibit even much longer lifetimes.

In the present work, we investigate this complex and the plain ligand by femtosecond TA spectroscopy and observe rich intramolecular relaxation dynamics. The shortest lifetime of 0.3 ps can be assigned to a flattening of the geometrical structure of the complex after optical excitation. The second exponential component of 3.3 ps reflects probably ISC to a triplet MLCT-state. However, the associated spectral signatures decay with a time constant of 10 ps. This may point to a transfer of the excited electron from the MLCT-state to a LC-state.

MO 6.2 Thu 14:15 H2

Ultrafast 2D-IR spectroscopy probes tRNA-Magnesium contact ion pairs — ●JAKOB SCHAUSS, ACHINTYA KUNDU, BENJAMIN P. FINGERHUT, and THOMAS ELSAESSER — Max Born Institute for Nonlinear Optics and Short-Pulse Spectroscopy, Berlin, Germany

The negative charge of nucleic acids makes them susceptible to interactions with their surrounding water shell and the ions embedded within. Magnesium ions in particular are known to strongly interact with RNA molecules, for example in the folding of functional RNA from an elongated chain into the native, condensed form. The interactions that play a role in the folding process are highly debated, partially due to the lack of non-invasive probes on the microscopic level.

Here, we use femtosecond 2D-IR spectroscopy of phosphate backbone vibrations to investigate the formation of transfer RNA/Mg²⁺ contact ion pairs (CIP). Phosphate vibrations have been shown to sense changes in the water environment upon RNA melting [1] and report on CIP formation in model systems [2]. The experimental results

on tRNA agree well with molecular dynamics simulations that show stabilization of tRNA tertiary structure through contact ion pairs. Particularly in highly congested regions of the tRNA, the magnesium ions are instrumental in efficiently compensating the high negative charge density [3].

[1] A. KUNDU *et al.*: *J. Phys. Chem. B*, 124, 2132-2138 (2020)

[2] J. SCHAUSS *et al.*, *J. Phys. Chem. Lett.* 10, 6281-6286 (2019)

[3] J. SCHAUSS *et al.*: *J. Phys. Chem. B*, 125, 740-747 (2021)

MO 6.3 Thu 14:30 H2

Unraveling collective coordinates influencing time-resolved x-ray absorption spectra of ionized urea and its dimer through machine learning — ●YASHOJ SHAKYA^{1,2}, LUDGER INHETER¹, CAROLINE ARNOLD^{1,2,3}, RALPH WELSCH^{1,3}, and ROBIN SANTRA^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY, Hamburg, Germany — ²Department of Physics, Universität Hamburg, Hamburg, Germany — ³Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Probing the early dynamics of chemical systems following ionization is essential for our understanding of radiation damage. Time-resolved x-ray absorption spectroscopy (TRXAS) on a femtosecond timescale can provide crucial insights into the ultrafast processes occurring upon ionization due to its element-specificity. However, even with theoretical simulations, getting a clear interpretation of the spectra can be challenging due to the high dimensionality of the data.

In this theoretical study, we investigate the response of urea and its dimer to ionizing radiation and how it can be probed via TRXAS. We show how statistical analysis techniques, in particular partial least square regression, can unravel specific structural dynamics in a molecule that induce changes in its TRXAS. By applying this technique, collective coordinates that most influence TRXAS are obtained from simulated ab initio nonadiabatic trajectories of valence-ionized urea and its dimer. For urea, this leads to the possibility of tracing specific molecular vibrations in its TRXAS. For its dimer, where ionization triggers a proton transfer, we show how the spectra can reveal the progress of the transfer.

MO 6.4 Thu 14:45 H2

Increasing ion yield CD in femtosecond photoionization of a prototypical chiral molecule using Optimal Control Theory — ●MANEL MONDELO-MARTELL, DANIEL BASILEWITSCH, CHRISTIANE P. KOCH, and DANIEL M. REICH — Freie Universität Berlin, Berlin, Germany

Molecular chirality is the property of some chemical compounds to have non-superimposable mirror images - enantiomers. These isomers in-

teract identically with non-chiral probes, but show different behaviour when subjected to chiral objects, thus the characterization and separation of enantiomers is both complex and very relevant. A particularly fundamental characterization technique is the so-called circular dichroism (CD), i.e. the difference in absorption of circularly polarized light by the two enantiomers.

CD with monochromatic light is usually a weak effect since it relies on differences in the magnetic transition dipole moments of the enantiomers. Previous work[1] qualitatively showed that shaping the light probes can affect the absorption profile of two enantiomers. Here, we use Optimal Control Theory to maximise the CD signal of the $A \leftarrow \pi^*$ transition in fenchone. Since this transition is dipole forbidden, we can use the interplay of multipolar interaction terms as a resource for the pulse optimization. We show that CD of oriented ensembles can be increased up to a 100% by selectively exciting the electronic state of only one enantiomer. We also get a significant increase when including orientational averaging for fenchone molecules in the gas phase.

[1] D. Kröner, J. Phys. Chem. A 115, 14510 (2011).

MO 6.5 Thu 15:00 H2

Is CCSD(T) a proper standard for dipole moment calculations? An analysis considering diverse diatomic species — ●XIANGYUE LIU¹, LAURA MCKEMMISH², and JESÚS PÉREZ-RÍOS¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — ²School of Chemistry, UNSW Sydney, Sydney, NSW 2052, Australia

Coupled cluster with single, double, and perturbative triple excitations [CCSD(T)] is considered one of the most accurate electronic structure methods and has been widely used as a reference in benchmarking studies. The present work investigates the accuracy of CCSD(T)

reproducing experimental ground state electric dipole moments and equilibrium distances of diatomic molecules. The results show that core-correlations are essential to some molecules, e.g., bi-alkali and main-group metal halides, to reach a satisfactory agreement with experimental measurements. However, for dipole moments of molecules involving transition metal atoms, CCSD(T) is not accurate enough even when including core-correlations. In addition, our work shows the relevance of using experimental data to benchmark theoretical quantum chemistry methods.

MO 6.6 Thu 15:15 H2

The Kicked Rotor and its Metrics of Chaos — ●CIAN HAMILTON and JESÚS PÉREZ RÍOS — Fritz Haber Institute, Berlin, Germany

The kicked rotor is a prototypical simple model that encompasses both order and chaos in classical and quantum variants. As a result, it has been extensively studied, although it is still not yet fully understood.

We have conducted a numerical exploration into both the classical and quantum kicked rotor, although from a different approach. As a result, we find that the transition from order to the chaos of the classical kicked rotor follows a hyperbolic tangent function depending on the kick strength by characterising the fractal dimension of the phase-space.

On the quantum front, we have been able to find how the localisation length for the wavefunction depends on the two quantum parameters controlling the system's dynamics. Similarly, by looking into the average kinetic energy after many kicks, we expect to have some hints about the emergence of quantum chaos and its correspondence with the classical dynamics. Finally, we have explored other areas of the kicked rotor, including how sensitive the system is to the dynamic kick period and dynamic kick strength.

MO 7: Poster 1

Time: Thursday 17:30–19:30

Location: P

MO 7.1 Thu 17:30 P

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

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

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

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

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

MO 7.2 Thu 17:30 P

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

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

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

MO 7.3 Thu 17:30 P

Dynamics of photo-excited cesium atoms attached to helium nanodroplets — ●N. RENDLER¹, A. SCOGNAMIGLIO¹, M.

BARRANCO^{2,3}, M. PÍ^{2,3}, N. HALBERSTADT⁴, K. DULITZ¹, and F. STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg — ²Departament FQA, Faculty of Physics, University of Barcelona — ³Institute of Nanoscience and Nanotechnology, University of Barcelona — ⁴Laboratoire des Collisions, Agrégats, Réactivité, Paul Sabatier University

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

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

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

[3] Rendler et al., arXiv:2106.12330

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

MO 7.4 Thu 17:30 P

Probing of a vibrational wave packet in the electronic ground state of methyl p-tolyl sulfoxide via time-resolved photoelectron circular dichroism — ●NICOLAS LADDA¹, MAX WATERS², VÍT SVOBODA², MIKHAIL BELOZERTSOV², SUDHEENDRAN VASUDEVAN¹, SIMON RANECKY¹, TONIO ROSEN¹, SAGNIK DAS¹, JAYANTA GHOSH¹, HANGYEOL LEE¹, HENDRIKE BRAUN¹, THOMAS BAUMERT¹, HANS JAKOB WÖRNER², and ARNE SENFTLEBEN¹ — ¹Institut für Physik, Universität Kassel, 34132 Kassel, Germany — ²Laboratorium für Physikalische Chemie, ETH Zürich, 8093Zürich, Switzerland

The dynamic change of the chiral character upon the laser-induced

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

MO 7.5 Thu 17:30 P

Chirp and intensity dependence of the circular dichroism in ion yield of 3-methylcyclopentanone measured with femtosecond laser pulses — ●SAGNIK DAS, JAYANTA GHOSH, TOM RING, SUDHEENDRAN VASUDEVAN, HANGYEOL LEE, NICOLAS LADDA, SIMON RANECKY, TONIO ROSEN, ARNE SENFTLEBEN, THOMAS BAUMERT, and HENDRIKE BRAUN — Institut für Physik, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

One of the methods to differentiate between the two enantiomers of a chiral molecule is Circular Dichroism (CD). It arises due to the difference in absorption of left and right circularly polarised light. The difference in absorption can also be mapped to the difference in ionisation of the enantiomers and is known as CD in ion yield[1,2]. We use our home-built Time of Flight (ToF) mass spectrometer with our recently established twin peak[3] measurement setup to study the effect of linear chirp (GDD) on the anisotropy. The candidate molecule for this experiment is 3-methylcyclopentanone (3-MCP). In the study we present here, we perform all the experiments at 309 nm, where 3-MCP shows high anisotropy, upto 10%. At this wavelength, a 1+1+1 resonance-enhanced multi-photon ionisation (REMPI) takes place in 3-MCP through the $\pi^* \leftarrow n$ transition. We observe enhancement of anisotropy for chirped pulses, which we compare to band-width limited pulses of equal peak intensity.

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

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

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

MO 7.6 Thu 17:30 P

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

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

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

MO 7.7 Thu 17:30 P

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

burg, Germany

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

MO 7.8 Thu 17:30 P

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

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

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

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

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

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

MO 7.9 Thu 17:30 P

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

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

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

MO 7.10 Thu 17:30 P

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

Ru^{II}-polypyridyl complexes are featured in a wide range of applications in the areas of medicine (photoactivatable prodrugs) and material science (photovoltaics/catalysis). Tailored ligand design enables the control of their efficiency and photoactivity by tuning the relative

energies of the $^3\text{MLCT}$ and ^3MC states. A selected series of Ru^{II} -polypyridyl complexes in the type of $[\text{Ru}(\text{y-bpy})_2(\text{x-py})_2]^{2+}$ ($\text{bpy} = (2,2\text{-bi})\text{pyridine}$), where x/y are varying substituents of different electronic donating/withdrawing character, were examined by a combination of mass spectrometry and laser spectroscopy in the frequency and time domain in an ion trap. Here, static absorption spectra were recorded by determining fragment ion yields as a function of laser wavelength (UV photodissociation spectra) and compared to TD-DFT calculations to characterize the electronic transitions. The femtosecond dynamics were elucidated via a pump-probe scheme recording excited-state lifetimes. Electron withdrawing substituents on the pyridine chromophore were found to destabilize the Ru^{II} -pyridine bond in the ground-state while stabilizing electronically excited-state ^3MC . Electron-donating substituents on bpy are observed to stabilize the coordinative bond, while stabilizing the $^3\text{MLCT}$ -state resulting in longer excited-state lifetimes.

MO 7.11 Thu 17:30 P

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

Multimetallic coinage metal complexes, featuring intricate metal-philic (M-M) interaction that govern photophysical properties such as bright luminescence and redox reactivity, are a prominent topic in functional material research [1,2]. Here, using quadrupole ion trap mass spectrometry, *in situ* synthesized homo- and heterobinuclear d^{10} - d^{10} metal complexes of type $[\text{MM}'(\text{dcpm})_2]^{2+}$ ($\text{M}, \text{M}' = \text{Cu}^{\text{I}}, \text{Ag}^{\text{I}}, \text{Au}^{\text{I}}$; $\text{dcpm} = \text{bis}(\text{dicyclohexylphosphino})\text{methane}$) were investigated in gas-phase via collisional-induced dissociation (CID) and ultraviolet photodissociation (UV PD) spectroscopy using femto- and nanosecond laser sources [3]. The resulting photodissociation spectra show a spectral blue shift of the lower energy metal-centered (MC) states in the order of $\text{Cu}_2 < \text{CuAu} < \text{CuAg} < \text{Au}_2 < \text{AgAu} < \text{Ag}_2$. These spectra were supported by quantum chemical calculations of *GW*-Bethe-Salpeter-equation (*GW*-BSE) approach, revealing a shortening of metal-metal binding upon excitation assigned to $^1\text{MC}(\text{d}\sigma^* \rightarrow \text{p}\sigma / \text{d}\sigma^* \rightarrow \text{p}\pi)$ transitions.

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

MO 7.12 Thu 17:30 P

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

Interstellar dust plays a major role in the formation processes of stars and solar systems. The formation mechanisms of this dust are, however, still poorly understood. One molecular species found in interstellar matter is SiO [1] and we try to understand how and if such small Si and O containing molecules can play a role in the formation of large μm -sized silicate particles, a major component of interstellar dust [2]. In this study we focus on silicon-oxide species with two oxygen atoms per molecule. The investigated cations are generated by a laser vaporization source and their mass spectra are examined [3]. We furthermore gain insight into the molecular structure and the electronic properties of Si_nO_2^+ s by measuring their photon energy dependent photodissociation behaviour which is compared to quantum chemical TD-DFT calculations.

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

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

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

MO 7.13 Thu 17:30 P

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

The ionization of randomly oriented chiral molecules with circularly polarized light leads to an asymmetric angular photoelectron distri-

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

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

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

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

MO 7.14 Thu 17:30 P

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

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

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

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

MO 7.15 Thu 17:30 P

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

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

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

MO 7.16 Thu 17:30 P

Magnetic properties and their correlation to the electronic ground states of isolated trinuclear 3d spin frustrated complexes — ●MICHAEL LEMBACH¹, JOHANNES LANG¹, MAXIMILIAN LUCZAK¹, YANNICK MEES¹, ROUMANY ISRAÏL¹, VICENTE ZAMUDIO-BAYER², MARTIN TIMM², CHRISTINE BÜLOW², BERND VON ISSEENDORFF⁴, AKIRA TERASAKI³, CHRISTOPH RIEHN¹, TOBIAS LAU², and GEREON NIEDNER-SCHATTEBURG¹ — ¹Technische Universität Kaiserslautern, Kaiserslautern, Germany — ²Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — ³Kyushu University,

Fukuoka, Japan — ⁴Physikalisches Institut, Freiburg, Germany

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

MO 7.17 Thu 17:30 P

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

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

MO 7.18 Thu 17:30 P

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

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

MO 7.19 Thu 17:30 P

Focused beams of small (bio-)nanoparticles from aerodynamic lens injectors — •LENA WORBS^{1,2}, JANNIK LÜBKE^{1,2,3}, AMIT K. SAMANTA¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg

Determining structure and observing dynamics from isolated proteins and nanoparticles using x-ray diffractive single-particle imaging (SPI) requires sample-delivery and injection methods that provide one single particle per x-ray pulse in the interaction region. Aerodynamic-lens-stack (ALS) injectors have been used to deliver collimated and

focused particle-beams for such experiments on larger nanoparticles (~50-100 nm) [1]. We extended the use and detection of particle beams toward smaller nanoparticles and present simulations and experiments on the performance of ALS injectors for 25 nm polystyrene spheres. This highlights the use of ALS injectors for small bio-nanoparticles. In addition, we present techniques to separate particles [2] according to charge caused by the aerosolization method employed. This paves the way toward pure beams of identical particles for SPI experiments.

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

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

MO 7.20 Thu 17:30 P

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

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

MO 7.21 Thu 17:30 P

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

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

MO 7.22 Thu 17:30 P

Mid-IR Photo-induced Dissociation of Solvated (Bio)Molecular Complexes — •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, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Center for Ultrafast Imaging, Universität Hamburg — ³Department of Physics, Universität Hamburg

We present the ultrafast imaging of thermal-energy chemical dynamics of micro-solvated (bio)molecular complexes when probing with strong-field techniques. We produce a pure sample of the molecule of interest in the gas phase by using a combination of a molecular beam and electrostatic deflector [1]. To study the thermally-induced dy-

namics, we set up a mid-IR pump-probe experiment, in which a 3 μm beam was used to excite the system and then a 1.3 μm nm beam was used for ionising the system. First experiments focus on the ion-imaging of the mid-IR pumped system. Future experiments will use laser-induced electron diffraction (LIED) [2,3] to probe the thermally-induced dynamics and obtain structural information about the system with atomic resolution.

- [1] S. Trippel, et al., *Rev. Sci. Instrum.* **89**, 096110 (2018).
- [2] J. Wiese, et al., *Phys. Rev. Research* **3**, 013089 (2021).
- [3] E. T. Karamatskos, et al., *J. Chem. Phys.* **150**, 244301(2019).

MO 7.23 Thu 17:30 P

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

Beyond the typical solid, liquid, and gaseous states of matter, certain materials exhibit mesophase properties, combining attributes of those categories. Liquid crystals (LCs), as a common example, show both solid-like order and fluid-like flow. So far, dynamics occurring within picosecond timescales in LCs are largely unexplored. They show resonant features in the THz spectral region [1], but a clear understanding of these signatures has yet to be developed. Here, we use few cycle THz pulses, generated via optical rectification in the organic crystal DSTMS, to perform both time-domain spectroscopy and resonant time-resolved birefringence measurements on various members of the nCB family of liquid crystals. The measured absorption spectra for uniformly aligned 5CB and 8CB, presenting nematic and smectic A phase, respectively, clearly indicate activity in the THz region. The THz induced birefringence associated with this activity shows oscillatory behaviour after the exciting pulse and thermalization within a few picoseconds. Our time resolved investigation includes depen-

dences on THz-field strength, pump and probe polarization independently controlled with respect to the LC alignment, and temperature, covering phase transitions. Interpretation and attribution to intra- or inter-molecular origin of the data is supported by gas phase theoretical calculations. [1] Vieweg, N., et al., *Optics Express*, 2012. 20(27)

MO 7.24 Thu 17:30 P

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

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

MO 8: Cold Molecules

Time: Friday 10:45–12:45

Location: H1

MO 8.1 Fri 10:45 H1

Quantum-state-controlled Penning collisions of ultracold lithium atoms with metastable atoms and molecules — ●TOBIAS SIXT, JIWEN GUAN, JONAS GRZESIAK, MARKUS DEBATIN, FRANK STIENKEMEIER, and KATRIN DULITZ — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Germany

In our experiment, we study quantum-state-controlled Penning collisions between laser-cooled lithium atoms (Li) and metastable helium atoms (He^*) to investigate new ways of controlling the outcome of Penning-ionizing collisions. In this contribution, we report on the efficient suppression of He^* -Li Penning ionization by laser excitation of the Li atoms. The results illustrate that not only the electron spin, but also Λ - the projection of the total molecular orbital angular momentum along the internuclear axis - is conserved during the ionization process. Our findings suggest that Λ conservation can be used as a more general means of reaction control, for example, to improve schemes for the simultaneous laser cooling and trapping of ultracold He^* and alkali atoms.

Furthermore, we report on the sensitive detection of metastable nitric oxide molecules, produced in a supersonic beam source, by reactive collisions with electronically excited Li atoms in the $2^2P_{3/2}$ state. We infer densities of $\approx 600 \text{ NO}(a^4\Pi_i)$ molecules/ cm^3 in the interaction region. Our results also allow for an estimate of the fractional population of $\text{NO}(a^4\Pi_i, v \geq 5)$ prior to the collision process.

MO 8.2 Fri 11:00 H1

Formation of van der Waals molecules in buffer gas cells through direct three-body recombination — ●MARJAN MIRAHMADI¹ and JESÚS PÉREZ-RÍOS^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — ²Department of Physics, Stony Brook University, Stony Brook, New York 11794, USA

We study the formation of van der Waals (vdW) molecules through direct three-body recombination processes $A + B + B \rightarrow AB + B$. In particular, the three-body recombination rate at temperatures relevant for buffer gas cell experiments is calculated via a classical tra-

jectory method in hyperspherical coordinates [*J. Chem. Phys.*, **140**, 044307 (2014)]. Furthermore, investigating the role of pairwise long-range interactions between the atoms involved, we could establish an exact threshold law for the formation rate of vdW molecules as a function of long-range dispersion coefficients of the pairwise interactions [arXiv:2107.02048 (2021)]. To study some examples we focus on the formation of vdW molecules X-RG (where RG is a rare gas atom) via $X + \text{RG} + \text{RG} \rightarrow X\text{-RG} + \text{RG}$ collisions [*J. Chem. Phys.*, **154**, 034305 (2021)]. As a result, we show that almost any X-RG molecule should appear in a buffer gas cell under appropriate conditions. It is pretty remarkable that, despite the drastic differences in the properties of the atom, X, and parameters of X-RG interaction potentials, the recombination rates are of the same order of magnitude.

MO 8.3 Fri 11:15 H1

Towards Transversal Laser Cooling of Barium Monofluoride — RALF ALBRECHT, MARIAN ROCKENHÄUSER, ●FELIX KOEGL, SINA HAMMER, PHILLIP GROSS, and TIM LANGEN — 5. Physikalisches Institut and Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Cold molecular gases are the starting point for many novel and interdisciplinary applications ranging from few- and many-body physics to cold chemistry and precision measurements. In particular, heavy polar molecules, such as barium monofluoride (BaF), are promising candidates for tests of fundamental symmetries and studies of quantum systems with strong, long-range interactions. Here, we report on our progress towards transversal cooling of an intense beam of such BaF molecules and discuss strategies for cooling of both bosonic and fermionic isotopologues.

MO 8.4 Fri 11:30 H1

Towards Zeeman slowing of Molecules — MARIA STEPANOVA, ●PAUL KAEBERT, TIMO POLL, MAURICE PETZOLD, SUPENG XU, MIRCO SIERCKE, and SILKE OSPELKAUS — Institute of Quantum Optics, Leibniz University Hannover

Ultracold molecules are a promising tool for studying fundamental physics, realizing novel states of matter, and investigating chemical

reactions with unprecedented control. Currently the field of ultracold molecules is making great experimental progress in these areas, but experiments using direct laser cooling of molecules remain limited by the number of ultracold particles they have access to. To increase this number, we have proposed a novel slowing method for molecules, reminiscent of the Zeeman slower for atoms. Here, we present our progress towards realizing such a molecular Zeeman slower. We show results from our recent characterization of the slowing force by measuring the photon scattering rate of a molecular beam moving perpendicular to the Zeeman slowing lasers. This configuration gives us a very narrow velocity-spread of the molecules, enabling us to extract the velocity dependence of the force. Our measurements are in excellent agreement with a simple rate equation model and demonstrate that the resulting force profile is capable of compressing the molecular velocity distribution from a standard buffer gas cell down to velocities necessary for trapping in a Magneto-optical Trap (MOT).

MO 8.5 Fri 11:45 H1

Buffer gas cooling and optical cycling of AlF molecules — ●SIMON HOFSSÄSS¹, MAXIMILIAN DOPPELBAUER¹, SID WRIGHT¹, SEBASTIAN KRAY¹, BORIS SARTAKOV², JESÚS PÉREZ-RÍOS¹, GERARD MEIJER¹, and STEFAN TRUPPE¹ — ¹Fritz Haber Institute of the Max Planck Society, Berlin, Germany — ²Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia

Aluminium monofluoride (AlF) is a promising candidate for a high-density magneto-optical trap (MOT) of molecules. Here, we show that AlF can be produced efficiently in a bright, pulsed cryogenic buffer gas beam, and demonstrate rapid optical cycling on the Q rotational lines of the $A^1\Pi \leftrightarrow X^1\Sigma^+$ transition at 228nm. We measure the brightness of the molecular beam to be $>10^{12}$ molecules per steradian per pulse in a single rotational state and present a new method to determine its velocity distribution accurately in a single molecular pulse. The photon scattering rate is measured using three different methods and compared to theoretical predictions of the optical Bloch equations and a rate equation model. An exceptionally high scattering rate of up to $42(7) \times 10^6 \text{ s}^{-1}$ can be sustained despite the large number of Zeeman sublevels (up to 216 for the Q(4) transition) involved in the optical cycle. We demonstrate that losses from the optical cycle due to vibrational branching to $X^1\Sigma^+$, $v=1$ can be addressed efficiently with a repump laser, allowing us to scatter about 10^4 photons using two lasers. Further, we investigate two other loss channels, photo-ionisation and parity mixing by stray electric fields. The upper bounds for these effects are sufficiently low to allow loading the molecules into a MOT.

MO 8.6 Fri 12:00 H1

An open microwave resonator for trapping ultracold polar molecules — ●MAXIMILIAN LÖW, FABIAN SALAMON, MARTIN IBRÜGGER, and MARTIN ZEPPENFELD — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

In recent years tremendous progress has been made producing polar molecules in the ultracold regime via direct cooling methods. However, one of the main challenges remains the realization of high phase space densities.

To this end, we are designing a microwave trap as the next stage in our experiment. Working at a frequency of 50 GHz it acts as a red-detuned dipole trap on the rotational transition $|J,K_a,K_c\rangle = |211\rangle \leftarrow |110\rangle$ of formaldehyde. We present the successful realisation of a high-finesse open microwave resonator to achieve trap depths above 1 mK with reasonable input power while maintaining optical access. Special focus is laid on a new type of incoupling mirror whose design was optimized using FEM simulations. It enables free-space coupling

into the resonator and is designed to dissipate tens of Watts of microwave power while its absorption losses stay small. To characterize our system, we developed special measurement techniques to determine the transmission through the incoupling mirror and the finesse of the resonator. First results show we can achieve a critically coupled finesse of at least 1650 with values of up to 2000 being in reach.

The resonator we developed fulfills the requirements to be used as a microwave trap for formaldehyde allowing us to aim for the regime of quantum degeneracy using evaporative or sympathetic cooling.

MO 8.7 Fri 12:15 H1

Generating degenerate $^{23}\text{Na}^{40}\text{K}$ molecules through a quantum phase transition — ●MARCEL DUDA, XING-YAN CHEN, ANDREAS SCHINDEWOLF, ROMAN BAUSE, RICHARD SCHMIDT, JONAS VON MILCZEWSKI, IMMANUEL BLOCH, and XIN-YU LUO — Max-Planck-Institut für Quantenoptik, Garching, Germany

A decade after the first creation of bi-alkali polar molecules, reaching quantum degeneracy remains a challenge even when associating a degenerate mixture of atoms. Starting from a mixture of bosonic and fermionic atoms, the bottleneck lies in the efficient association of weakly-bound Feshbach molecules. The density mismatch, severe loss, and consequent heating prevent the exploration of the Bose-Fermi mixture in the strongly interacting regime and, thus, the Feshbach association. We eliminate the detrimental loss by decompressing a Bose-Einstein condensate (BEC) of sodium to density-match it with a degenerate Fermi gas of potassium. By doing so, we can associate 50000 long-lived $^{23}\text{Na}^{40}\text{K}$ Feshbach molecules below 0.3 of the Fermi temperature. We characterize the association through the depletion of the condensate fraction and observe a good agreement with theoretical predictions of a phase transition from polarons to molecules. The degeneracy is underlined by partially restoring a BEC when reversing the association ramp. In the last step, we produce 30000 $^{23}\text{Na}^{40}\text{K}$ polar molecules at an effective temperature of half the Fermi temperature.

MO 8.8 Fri 12:30 H1

Towards the Ultracold Dipolar Quantum Gas of $^6\text{Li}^{40}\text{K}$ — ●ANBANG YANG¹, SOFIA BOTSIS¹, SUNIL KUMAR¹, VICTOR ANDRE AVALOS PINILOS¹, CANMING HE^{1,2}, and KAI DIECKMANN^{1,2} — ¹Centre for Quantum Technologies, 3 Science Drive 2, Singapore 117543 — ²Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542

We demonstrate a two-photon pathway to the rovibrational ground state of $^6\text{Li}^{40}\text{K}$ molecules that involve only singlet-to-singlet transitions. We start from a Feshbach state which contains a significant singlet character of 52%. With the only contributing singlet state to the molecular state being fully stretched and with control over the polarization of the laser we address a sole hyperfine component of the $A^1\Sigma^+$ potential without resolving its hyperfine structure. The dark resonance spectroscopy is performed with two narrow-linewidth lasers to precisely determine the two-photon resonance for STIRAP transfer to the $v'' = 0$ ground state. The strong dipolar nature of ground state $^6\text{Li}^{40}\text{K}$ is revealed by Stark spectroscopy. A high finesse cavity is built to simultaneously stabilize the two STIRAP lasers using the PDH lock to ensure relative phase coherence. Apart from the narrow linewidth, the phase noise of lasers is also crucial for coherent population control. We characterize the phase noise of the STIRAP laser system and estimate the loss during the population transfer. Several improvements have been made to suppress the excessive phase noise. The estimation based on the new noise characterization promises for the low loss STRIAP to the ground state.

MO 9: Poster 2

Time: Friday 17:30–19:30

Location: P

MO 9.1 Fri 17:30 P

LiK $B^1\Pi$ potential: combining short and long range data — ●SOFIA BOTSIS¹, ANBANG YANG¹, SAMBIT B. PAL¹, MARK M. LAM¹, SUNIL KUMAR¹, MARKUS DEBATIN¹, and KAI DIECKMANN^{1,2} — ¹Centre for Quantum Technologies (CQT), 3 Science Drive 2, Singapore 117543 — ²Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542

We report on high-resolution spectroscopic measurements of the long-

range states of the $^6\text{Li}^{40}\text{K}$ molecule near the $^6\text{Li}(2^2S_{1/2})+^{40}\text{K}(4^2P_{3/2})$ dissociation threshold, which in combination with existing data in the short-range lead to the complete characterization of the $B^1\Pi$ potential. Starting from weakly bound ultracold Feshbach molecules, we perform one-photon loss spectroscopy of the $B^1\Pi$ and record the transition frequencies to twenty-five vibrational levels. Level assignment to the spin-orbit coupled potentials is facilitated by existing data in the long-range and by examining the Zeeman effect for the Hund's case (c) coupling scheme. The C_6 coefficients are deduced by fitting our

vibrational energies together with the long-range levels to the LeRoy-Bernstein formula. We present a complete set of data for the $\Omega=1^{up}$ state, by combining the long-range measurements with data from the short-range states of the $B^1\Pi$ obtained for the $^7Li^{39}K$ isotopologue. Using mass-scaling, we model the short- and the long-range states simultaneously and produce an improved Rydberg-Klein-Rees curve for the complete potential. ¹Ridinger *et al.*, *EPL*, 2011, **96**, 33001, ²Pashov *et al.*, *Chem. Phys. Lett.*, 1998, **292**, 615-620

MO 9.2 Fri 17:30 P

New Lifetime Limit of the Ground State Vinylidene Anion H_2CC^- — ●FELIX NUSSLIN¹, KLAUS BLAUM¹, JÜRGEN GÖCK¹, MANFRED GRIESER¹, SEBASTIAN GEORGE², ROBERT VON HAHN¹, ÁBEL KÁLOSI^{3,1}, HOLGER KRECKEL¹, DAMIAN MÜLL¹, OLDŘICH NOVOTNÝ¹, HENRIK PEDERSEN⁴, VIVIANE SCHMIDT¹, and ANDREAS WOLF¹ — ¹Max-Planck-Institut für Kernphysik, Heidelberg, 69117, Germany — ²Institut für Physik, Universität Greifswald, Greifswald, 17487, Germany — ³Columbia Astrophysics Laboratory, Columbia University, New York, 10027, USA — ⁴Department of Physics and Astronomy, Aarhus University, Aarhus, 8000, Denmark

The isomers acetylene (HCCH) and vinylidene (H_2CC) form one of the simplest systems for studying isomeric reactions involving hydrogen. In anionic form the vinylidene isomer has the lowest total energy with an electron affinity of ~ 0.5 eV. It lies 1.5 eV above the lowest neutral level of acetylene, which gives rise to the hypothesis that isomerization linked with electron emission could limit the lifetime of H_2CC^- . An experiment at a room-temperature storage ring obtained a finite lifetime of ~ 110 s [1] by extrapolating from collision-limited (~ 10 s) to collision-free beam lifetimes of H_2CC^- and a stable reference ion. To access longer ion beam lifetimes (up to 3000 s) and thereby enable a better estimate of the ground state H_2CC^- lifetime, we employed the Heidelberg electrostatic Cryogenic Storage Ring [2]. From comparing the decays of H_2CC^- and the stable reference ion CN^- we find that the ground state H_2CC^- lives at least 3500 s, i.e., more than an order of magnitude longer than assumed previously. The latest results will be presented.

[1] M. Jensen *et al.*, *Phys. Rev. Lett.* 84 (2000) 1128.

[2] R. von Hahn *et al.*, *Rev. Sci. Instrum.* 87 (2016) 063115.

MO 9.3 Fri 17:30 P

Towards the coherent control of Penning collisions between metastable helium atoms — ●ALEXANDRA TSOUKALA, LASSE BINIKOWSKI, TOBIAS SIXT, NICOLAS VANHAECKE, FRANK STIENKEMEIER, and KATRIN DULITZ — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Our research focuses on understanding the mechanistic details of reactive collisions in order to enable control of their outcome. The coherent control of reactive collisions, which relies on the interference between two or more reaction paths, has been long sought for. We are in the process of realizing an experiment, in which we coherently control the Penning collisions between metastable helium atoms in 2^3S_1 and 2^1S_0 states.

Our control scheme is based on the preparation of a coherent superposition of the $M_J=-1$ and $M_J=+1$ quantum states in the $He(2^3S_1)$ via an off-resonant two-photon Rabi excitation scheme. The two states are coupled by light of counter-rotating circular polarization, which also imprints its phase onto each state. By varying the phase difference between the two circularly polarized light components, the relative phase between the involved reaction pathways follows the same trend. This control scheme will allow for a precise tuning of the overall reaction cross section. Our detection scheme is based on the monitoring of ions produced in the collision process using a time-of-flight detector.

In this contribution, I will describe our experimental apparatus and its characterization.

MO 9.4 Fri 17:30 P

A direct comparison of buffer gas molecular beams of AlF, CaF and MgF — ●MAXIMILIAN DOPPELBAUER, SIDNEY WRIGHT, XIANGYUE LIU, SIMON HOFSSÄSS, JESÚS PÉREZ-RÍOS, GERARD MEIJER, and STEFAN TRUPPE — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The production of dense, controlled samples is crucial for many applications of ultracold molecules. Cryogenic buffer gas sources are widely used for producing bright, slow beams of internally cold molecules. We aim to understand the formation process of the laser-coolable monofluorides AlF, CaF and MgF after laser ablation of a metal target and reaction with a fluorine donor gas. We combine theoretical calcula-

tions with a systematic experimental approach for this study.

We first examined the reaction rate for different reactants using molecular dynamics simulations. The electronic interaction energy was calculated on the fly using the BHLYP-D3 functional, and the def2-TZVP basis set. The calculations predict that AlF is produced more efficiently using NF_3 , than with SF_6 , and that the formation of AlF is one order of magnitude more efficient than that of CaF.

In the experiment, we measured the brightness of Al and Ca atomic beams and compared it to AlF, CaF and MgF molecular beams. We show that the AlF beam is one order of magnitude brighter than a CaF or MgF beam formed in the same buffer gas source, both in absorption and in fluorescence. The fact that the atomic beams of Al and Ca are similar in brightness supports the theoretical result. All atomic and molecular beams have similar forward velocity distributions.

MO 9.5 Fri 17:30 P

Ozone formation through three-body collisions: Theory and experiment reconciled — ●MARJAN MIRAHMADI¹, JESÚS PÉREZ-RÍOS^{1,2}, OLEG EGOROV³, VLADIMIR TYUTEREV^{3,4}, and VIATCHESLAV KOKOULINE⁵ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — ²Department of Physics, Stony Brook University, Stony Brook, New York 11794, USA — ³Quamer Laboratory, Tomsk State University, Tomsk, Russia — ⁴Groupe de Spectrometrie Moléculaire et Atmosphérique, UMR CNRS 7331, University of Reims Champagne-Ardenne, Reims, France — ⁵Department of Physics, University of Central Florida, Florida, USA

We present a direct three-body recombination approach to study the formation of ozone through the ternary collision $O_2 + O + M \rightarrow O_3 + M$, where M can be N_2 , O_2 or Ar. The rate coefficients for the formation of O_3 , without using two-steps approximations, were computed for the first time as a function of collision energy. Accordingly, thermally-averaged rates were derived for temperatures 5-900 K. As a result, we find that most of the ozone molecules are formed in weakly bound states that are further vibrationally quenched into deeply bound vibrational states relevant for UV absorption, in agreement with the experimental observations. Moreover, our formalism, based on classical trajectory calculations, allows having a fully *ab initio* and pressure-independent rate for ozone formation.

MO 9.6 Fri 17:30 P

State-selective cross sections from Ring PolymerMolecular Dynamics — ●ADRIEN MARJOLLET — CFEL-DESY, Hamburg, Germany

Understanding the influence of different forms of energy (e.g., translational, vibrational, rotational) on chemical reactions is a key goal and great challenge in physical chemistry. Very recently we proposed a new approach to obtain state-selective cross sections that approximately includes quantum effects like zero-point energy and tunneling. The method is a combination of the widely used quasiclassical trajectory approach (QCT) and the ring polymer molecular dynamics method (RPMD). The approach is then applied and assessed to several prototypical $X+H_2(\nu=0,1)$, $X=Mu, H, D, F, Cl$ and $H/F+CH_4$ reactions. Good agreement with rigorous quantum dynamics simulations is found for most cases.

MO 9.7 Fri 17:30 P

Quantitative detection of C_2H_2 in a dusty plasma environment using sensitive mid-IR frequency modulation spectroscopy — ●MITHUN PAL¹, MICHAEL STUHR¹, NANCY FASSHEBER¹, ANDREAS PETERSEN², FRANKO GREINER², and GERNOT FRIEDRICH¹ — ¹Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Germany — ²Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

We report both the implementation of single- and two-tone mid-IR frequency modulation (FM) schemes to measure acetylene (C_2H_2) concentration transients in a low-temperature dusty plasma arising from a RF discharge in low-pressure argon with C_2H_2 admixture. The key underlying concept of the FM technique is to shift the detection bandwidth of the optical spectrometer to a high-frequency region, where conventional technical noise from the laser source and experimental environment become negligible. Moreover, due to the derivative nature of the acquired spectra, broadband background absorption and scattering from interfering species or particles are efficiently suppressed. In order to quantify the concentration of acetylene, we experimentally probed the P(25)e rovibrational transition of C_2H_2 at 3233.08 cm^{-1} , originating from the fundamental vibrational band ν_3 (asymmetric C-H stretch). Additionally, we monitored the periodic C_2H_2 dynamics

under variable discharge conditions to demonstrate the high potential of transient mid-IR FM spectroscopy to gain insight into the kinetics of the nanoparticle nucleation, growth, and precipitation.

MO 9.8 Fri 17:30 P

Core-level intermolecular Coulombic decay in pyrimidine enabled by aqueous environment — •DANA BLOSS¹, CATMARNA KÜSTNER-WETEKAM¹, PHILIPP SCHMIDT¹, SASCHA DEINERT², FLORIAN TRINTER², GREGOR HARTMANN¹, ARNO EHRESMANN¹, LORENZ S. CEDERBAUM³, NIKOLEI V. KRZYZHEVOI³, ANDRÉ KNIE¹, and ANDREAS HANS¹ — ¹Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ²Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg — ³Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany

We investigated the effect of the presence or absence of an aqueous environment for bio-relevant molecules after their exposure to X-ray irradiation in a photoelectron-ion-ion coincidence experiment performed at the P04 at Petra III. In the decay of carbon inner-shell vacancies of hydrated pyrimidine we found evidence for direct intermolecular Coulombic decay. This process protects the molecule from reaching dicationic states via Auger decay and the inevitable fragmentation. The observations are compared with the results of theoretical calculations for a deeper understanding of the occurring effects.

MO 9.9 Fri 17:30 P

Ultrafast Spectroscopy of Perylene Derivative Nanoparticles — •CHRIS REHHAGEN¹, SHAHNAWAZ RAFIQ², KYRA N. SCHWARZ³, STEFAN LOCHBRUNNER¹, and GREGORY D. SCHOLES² — ¹Institute for Physics and Department of Life, Light and Matter, University of Rostock, 18051 Rostock, Germany — ²Frick Laboratory, Princeton University, 08540 Princeton, USA — ³School of Chemistry, University of Melbourne, Parkville, VIC, 3010 Australia

Organic nanostructures are of increasing interest in opto-electronic applications due to their potentially large exciton mobilities. While as inorganic nanoparticles are already applied in many scenarios, the properties of organic nanostructures are yet to be explored. Among a breadth of organic systems available, Perylene derivatives attract much interest as they provide a high oscillator strength, photostability, and a tuneability of the transition energy and supramolecular structure. We use flash precipitation to prepare nanoparticles of the dye Perylene Red and correlate their optical spectra, quantum yields and emission lifetimes. Ultrafast pump-probe spectroscopy is then performed on samples of different classes to characterize their excited state dynamics. An intermediate charge-transfer state, formed after photoexcitation, was observed. Remarkably, no such intermediate state was observed in the monomer of Perylene Red. We further characterize the exciton diffusion in the nanoparticles by analyzing signatures in the transient dynamics resulting from exciton-exciton annihilation. The resulting diffusion constant is 0.2 nm²/ps resulting in a diffusion length of 10 nm within the singlet exciton lifetime of 90 ps.

MO 9.10 Fri 17:30 P

Predicting *ortho-para* transitions of water from first principles — •GUANG YANG^{1,2}, ANDREY YACHMENEV^{1,3}, SERGEI YURCHENKO⁴, EMIL ZAK¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg — ⁴Department of Physics and Astronomy, University College London, UK

We present a complete room-temperature hyperfine-resolved line list of H₂¹⁶O, including forbidden *ortho-para* transitions. The predicted strongest forbidden *ortho-para* transition intensities are at the order of 10⁻³¹ cm/molecule, which is an order of magnitude stronger than the previous results. The calculations were based on the variational approach TROVE with including the hyperfine effects by nuclear spin-rotation and spin-spin interactions. The computed line list cover transitions between energy levels up to $F = 39$ ($J = 40$) and vibrational band centers up to 15000 cm⁻¹. The comparison between the calculated hyperfine transitions and the available experimental data shows good agreement. This line list will be useful for guiding future experimental spectroscopic studies of hyperfine structure and nuclear spin dynamics.

- [1] G. Yang, et al., *J. Chem. Phys.*, in preparation (2021)
- [2] S. N. Yurchenko, et al., *J. Mol. Spectrosc.*, **245**, 126 (2007)
- [3] A. Miani, et al., *J. Chem. Phys.*, **120**, 2732 (2004)
- [4] H. Bluysen, et al., *Phys. Lett. A*, **24**, 482 (1967)

[5] G. Cazzoli, et al., *Chem. Phys. Lett.*, **473**, 21 (2009)

MO 9.11 Fri 17:30 P

Statistical analysis of correlations in the x-ray induced Coulomb explosion of iodopyridine — BENOÎT RICHARD^{1,2,3}, •JULIA SCHÄFER^{1,4}, ZOLTAN JUREK¹, ROBIN SANTRA^{1,2,3,4}, and LUDGER INHETER^{1,2} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — ²The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — ³Department of Physics, Universität Hamburg, Notkestr. 9-11, 22607 Hamburg, Germany — ⁴Department of Chemistry, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Coulomb explosion imaging is a promising experimental tool to study individual molecules. However, the amount of information about the original molecule that can be retrieved from the measured final momenta of the produced ions is unclear. In particular, little study has been made about how to exploit information about the correlations between the ion momenta that state-of-the-art multi-coincidence techniques can acquire. In this work simulation data for the x-ray induced Coulomb explosion of 2-iodopyridine is analyzed and the involved fragmentation dynamics are described. It is found that particular final ion momenta show correlations that reflect a collision of two atoms during the explosion. Moreover covariances of the forces along the explosion can be utilized to simplify the description of the dynamics in reduced dimensionality using only four collective coordinates.

MO 9.12 Fri 17:30 P

Spectral deep-learning for (ro-)vibrational calculations of weakly-bound molecules — •JANNIK EGGERS^{1,2}, YAHYA SALEH^{1,2}, VISHNU SANJAY^{1,2,3}, ANDREY YACHMENEV^{1,3}, ARMIN ISKE², and JOCHEN KÜPPER^{1,3,4} — ¹Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Mathematics, Universität Hamburg — ³Center for Ultrafast Imaging CUI, Universität Hamburg — ⁴Department of Physics, Universität Hamburg

Planning and elucidating experiments on resonances in dissociation dynamics of molecules and molecular clusters requires accurate quantum mechanical calculations of (ro-)vibrational energies up to dissociation, which is a big challenge especially for larger molecules. Standard approaches represent wavefunctions as linear combinations of some fixed basis set and the quality of the predictions highly depends on the choice of the basis set. Furthermore, the computational costs scale poorly with the dimension of the problem.

We present a nonlinear neural network-based variational framework to simultaneously compute several eigenstates and eigenfunctions of the Hamiltonian. Unlike linear variational methods, neural network-based models seem to scale relatively well with the dimension of the problem. While they were mainly used to successfully model ground states of quantum systems, our approach extends to excited states. The key principle is to use neural networks as an adaptive basis and to optimize it, enabling us to use a much smaller basis set than in standard approaches without sacrificing accuracy.

MO 9.13 Fri 17:30 P

eCOMO - A new endstation for controlled molecule experiments — •WUWEI JIN¹, SEBASTIAN TRIPPEL^{1,3}, HUBERTUS BROMBERGER^{1,3}, TOBIAS RÖHLING¹, KAROL DLUGOLECKI¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg

We present details on our newly established transportable endstation eCOMO (Endstation for Controlled Molecules). The apparatus has been designed for use at various photon sources for investigating the molecular dynamics of small molecules in the gas phase [1].

The endstation consists of three main parts: 1) An Evan-Lavie-valve-based gas source. 2) An electrostatic deflector for the generation of pure molecular samples [2]. 3) A double-sided VMI spectrometer coupled with the time- and position sensitive Timepix3 camera [3].

The endstation was designed to be highly transportable, with built-in transport wheels, adjustable height, integrated controllers, power supplies as well as water and gas lines for easy beamtime installation. Here, we discuss our first results on the UV dissociation dynamics of carbonyl sulphide (OCS) [4].

- [1] M. Johny, J. Onvlee, et al., *Chem. Phys. Lett.*, **721**, 149 (2019)
- [2] S. Trippel, M. Johny, et al., *Rev. Sci. Instrum.*, **89**, 096110 (2018)

[3] A.F Al-Refai, M Johny, et al., *J. Instrum.*, **14**, P10003 (2019)

[4] In collaboration with the group of Francesca Calegari, within the Center for Molecular Water Science (CMWS)

MO 9.14 Fri 17:30 P

Method of Kinetic Energy Reconstruction from Ion-Time-of-Flight Spectra — ●AARON NGAI¹, KATRIN DULITZ¹, MARCEL MUDRICH², and FRANK STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — ²Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, 8000 Aarhus C

We present a method which makes use of ion trajectory simulations to reconstruct ion-kinetic-energy (KE) distributions from ion-time-of-flight (TOF) spectra. Sufficient conditions for a unique calibration to experimental parameters are presented, where the calibrated simulation extrapolates to a set of energy-dependent TOF basis functions, allowing conversion between TOF and KE coordinates. We demonstrate this reconstruction method on a recent XUV-UV pump-probe laser experiment on helium nanodroplets at the free-electron laser FERMI in Trieste [1], where relaxation from the 1s3p/1s4p droplet absorption band was time-resolved, using a Wiley-McLaren-type ion-TOF spectrometer in combination with a magnetic bottle electron spectrometer [2,3].

[1] J. D. Asmussen *et al.* *Phys. Chem. Chem. Phys.* advance article (2021).

[2] W. C. Wiley and I. H. McLaren. *Rev. Sci. Instrum.* **26**, 1150 (1955).

[3] J. H. Eland *et al.* *Chem. Phys.* **327**, 85 (2006).

MO 9.15 Fri 17:30 P

Coherent two-dimensional photoelectron spectroscopy — ●DANIEL UHL, ULRICH BANGERT, LUKAS BRUDER, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany.

Coherent multidimensional spectroscopy (CMDS) is probably the most complete spectroscopic technique to study couplings, coherence properties and real-time dynamics of a quantum system [1,2,3]. Another spectroscopic method is photoelectron spectroscopy which provides detailed information about the chemical composition and electronic states of the sample [4].

In our work we present a combination of both methods in a single experiment. This becomes feasible with the implementation of efficient single-counting detection and multichannel software-based lock-in amplification [5]. The approach offers high temporal, spectral and kinetic energy resolution. It enables differential CMDS experiments with unprecedented selectivity and enhances the dynamic range of CMDS by up to two orders of magnitude.

[1] D.M. Jonas, *Annu. Rev. Chem. Phys.* **54**, 425-463 (2003).

[2] R.M. Hochstrasser, *PNAS* **104**, 14190-14196 (2007).

[3] L. Bruder *et al.*, *Nat Commun* **9**, 4823 (2018).

[4] S. Hüfner, *Photoelectron Spectroscopy: Principles and Applica-*

tions (Springer Science & Business Media, 2013).

[5] D. Uhl, L. Bruder, and F. Stienkemeier, *ArXiv*, 2105.12124 (2021).

MO 9.16 Fri 17:30 P

Driving Waveform Dependency of Energy Dissipation of Trapped Particles — ●MARTIN KERNBACH^{1,2}, PAUL OSKAR SUND¹, and ANDREAS W. SCHELL^{1,2} — ¹Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — ²Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, D-38116 Braunschweig, Germany

Trapping is an beneficial tool for investigations on and experiments with ions or microparticles. Optical resonance and fluorescence probing of isolated microparticles are essential to determine their spectroscopic fingerprints which gives information about their structural properties or internal degrees of freedom. On the other hand trapped ions are used for quantum computing or atomic clocks by manipulating their quantum states with systematic laser-light interaction. Ions can be trapped by optical cooling techniques such as Doppler cooling, while microparticles mainly lose their energy due to atmospheric friction. Although both processes are based on a different physical background, the dynamic of both can be described by an energy dissipation term proportional to the velocity of the particle. We have simulated the trapping process for a better understanding of the underlying dynamics and to test different trapping optimization approaches, for example exotic driving waveforms respectively for single particle trapping and two particles in a sympathetic cooling scheme.

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Interplay of periodic dynamics and noise: insights from a simple adaptive system — ●FREDERIC FOLZ¹, KURT MEHLHORN², and GIOVANNA MORIGI¹ — ¹Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — ²Algorithms and Complexity Group, Max-Planck-Institut für Informatik, Saarland Informatics Campus, 66123 Saarbrücken, Germany

We study the dynamics of a simple adaptive system in the presence of noise and periodic damping. The system is composed by two paths connecting a source and a sink, the dynamics is governed by equations that usually describe food search of the paradigmatic *Physarum polycephalum*. In this work we assume that the two paths undergo damping whose relative strength is periodically modulated in time and analyse the dynamics in the presence of stochastic forces simulating Gaussian noise. We identify different responses depending on the modulation frequency and on the noise amplitude. At frequencies smaller than the mean dissipation rate, the system tends to switch to the path which minimizes dissipation. Synchronous switching occurs at an optimal noise amplitude which depends on the modulation frequency. This behaviour disappears at larger frequencies, where the dynamics can be described by the time-averaged equations. Here, we find metastable patterns that exhibit the features of noise-induced resonances.