MO 30: Poster – Molecular Spectroscopy

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

MO 30.1 Thu 17:00 Philo 1. OG

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

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

MO 30.2 Thu 17:00 Philo 1. OG

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

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

[1] Esteves-López et al., Phys. Chem. Chem. Phys. 18 (2016) 25637
[2] Liu et al., Chem. Phys. 464 (2016) 78

MO 30.3 Thu 17:00 Philo 1. OG

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

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

MO 30.4 Thu 17:00 Philo 1. OG

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

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

MO 30.5 Thu 17:00 Philo 1. OG

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

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

MO 30.6 Thu 17:00 Philo 1. OG

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

In aromatic radical cation dimers, charge resonance (CR), in which a positive charge is delocalized over both monomers, is one of the strongest forces with binding energies of $\sim$100 kJ/mol, favoring sandwich structures. The strength of CR depends strongly on the differences between the ionization energies (ΔIE) of the interacting monomers. Thus, homodimers such as the pyrrole dimer cation ($Py_2{}^+$) have the strongest CR. However, in heterodimers, CR is weakened, allowing other bonding motifs, such as $NH\cdots\pi$ H-bonding to compete, favoring T-shaped structures. Herein, we investigate the binding motifs of pyrrole$^+$-benzene (Py^+Bz), pyrrole$^+$-toluene (Py^+Tol), and pyrrole$^+$-naphthalene (Py^+Np) heterodimers, with ΔIE=1.03, 0.59, and -0.06 eV, respectively, using infrared photodissociation spectroscopy (IRPD) and density functional theory calculations. Analysis of IRPD spectra of mass-selected Py^+Bz, Py^+Tol, and Py^+Np, combined with geometric parameters of intermolecular structures, reveals that competition between NH$\cdots\pi$ H-bonding and CR interaction with respect to ΔIE of the monomers.

MO 30.7 Thu 17:00 Philo 1. OG

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

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

MO 30.8 Thu 17:00 Philo 1. OG

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

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

MO 30.9 Thu 17:00 Philo 1. OG

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

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

MO 30.10 Thu 17:00 Philo 1. OG

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

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

MO 30.11 Thu 17:00 Philo 1. OG

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

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

MO 30.12 Thu 17:00 Philo 1. OG

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

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

MO 30.13 Thu 17:00 Philo 1. OG

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

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

MO 30.14 Thu 17:00 Philo 1. OG

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

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

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

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

MO 30.15 Thu 17:00 Philo 1. OG

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

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

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

References:

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

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

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

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

MO 30.16 Thu 17:00 Philo 1. OG

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

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

MO 30.17 Thu 17:00 Philo 1. OG

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

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

MO 30.18 Thu 17:00 Philo 1. OG

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

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

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

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

MO 30.19 Thu 17:00 Philo 1. OG

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

We present our recently measured gas-phase photoelectron spectra (PES) of doped (cage-modified) diamondoids, namely 2-oxaadamantane, 2-thiaadamantane, and urotropine, to investigate the excited electronic states of their respective cations. These are interpreted with the aid of quantum chemical calculations and compared to the PES spectra of previously measured diamondoids. Heteroatom substitution within the carbon-cage network yields large band gaps between the ground and first excited states. Furthermore, vibronic fine structure is observed in the higher energy bands that is not observed in the spectra of the bare and functionalized diamondoids. Electronic photodissociation (EPD) spectroscopy reveals that in the case of urotropine^{+}, resolved vibronic structure attributed to the $\mathrm{D}_3(^2\mathrm{A}_1)\leftarrow\mathrm{D}_0(^2\mathrm{A}_1)$ electronic transition appears at a band origin of 29,990 cm^{-1} (333.4 nm) and grows increasingly more congested toward higher photon energy, suggesting considerable geometric distortion upon electronic excitation of the Jahn-Teller distorted ground electronic state. These measurements provide critical reference data for astronomical searches in the pursuit of a broader understanding of the chemical inventory of the interstellar medium.

MO 30.20 Thu 17:00 Philo 1. OG

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

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

MO 30.21 Thu 17:00 Philo 1. OG

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

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

MO 30.22 Thu 17:00 Philo 1. OG

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

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