# MO 27: Molecular Spectroscopy II

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

MO 27.1 Thu 14:30 P 204

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

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

MO 27.2 Thu 14:45 P 204

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

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

MO 27.3 Thu 15:00 P 204

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

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

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

MO 27.4 Thu 15:15 P 204

**Dissociative Single and Double Ionization of Thymine** — •Sitanath Mondal[1], Sitanath Mondal[1], Sitanath Mondal[2], Sitanath Mondal[2], Sitanath Mondal[1], and Sitanath Mondal[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Desirs Beamline, Synchrotron Soleil, St. Aubin, France

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

MO 27.5 Thu 15:30 P 204

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

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

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

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

MO 27.6 Thu 15:45 P 204

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

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

MO 27.7 Thu 16:00 P 204

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

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

MO 27.8 Thu 16:15 P 204

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

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