

MO 20: Poster III

Time: Thursday 16:30–19:00

Location: Empore Lichthof

MO 20.1 Thu 16:30 Empore Lichthof

Photoelectron Circular Dichroism of fenchone induced by coherent broadband laser pulses — ●ERIC KUTSCHER, ANTON ARTEMYEV, and PHILIPP DEMEKHIN — Institut für Physik und CIN-SaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Angular distributions of photoelectrons ionized by circularly polarized light from randomly oriented chiral molecules are asymmetric with respect to the propagation direction of the light [1]. This Photoelectron Circular Dichroism (PECD) appears also in the multiphoton ionization regime [2], which opens up a possibility for the coherent control of the effect. So far, the quantum control of PECD has only been discussed in a pump-probe excitation scheme with narrowband pulses [3]. Broadband (bb) laser pulses support photons in a large energy interval [4] and can be tailored in their amplitude and phase with pulse-shaping techniques. Here, the multiphoton PECD induced by coherent bb pulses with a 1-3 eV energy spectrum is studied theoretically for R(-)-fenchone molecules with different chirps and intensities of the pulses by utilizing the time-dependent single-center method [5]. Our results confirm a possibility to control the multiphoton PECD by tailored coherent bb pulses.

- [1] B. Ritchie, *Phys. Rev. A* **13**, 1411 (1976).
- [2] C. Lux *et. al.*, *Angew. Chem. Int. Ed.* **51**, 5001 (2012).
- [3] R. E. Goetz *et. al.*, *Phys. Rev. Lett.* **122**, 013204 (2019).
- [4] H. Hundertmark *et. al.*, *Opt. Express* **17**, 1919 (2009).
- [5] A.N. Artemyev *et. al.*, *J. Chem. Phys.* **142**, 244105 (2015).

MO 20.2 Thu 16:30 Empore Lichthof

Nondipole-Induced Asymmetry in the photoelectron emission distribution from fixed-in-space CO molecules — ●DMITRII REZVAN¹, KIM KLYSSEK², SVEN GRUNDMANN², ANDREAS PIER², NIKOLAY NOVIKOVSKIY¹, NICO STRENGER², DIMITRIOS TSITSONIS², MAX KIRCHER², ISABEL VELA-PEREZ², KILIAN FEHRE², FLORIAN TRINTER², MARKUS SCHÖPFLE², TILL JAHNKE², REINHARD DÖRNER², and PHILIPP DEMEKHIN¹ — ¹Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Institut für Kernphysik, J.W. Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

A nondipole-induced asymmetry in the angular distributions of C and O 1s-photoelectrons of fixed-in-space CO molecules is studied experimentally and theoretically at a photon energy of 905 eV. We demonstrate how scattering and nondipole effects determine the final emission distributions. The calculations were carried out in the frozen-core Hartree-Fock approximation using the stationary single center method [1], while the experiment was carried out using the COLTRIMS reaction microscope [2] available at beamline P04 of PETRA III, DESY. The emission distributions possess a strong scattering peak in the direction of the neighboring atom. This peak is either enhanced or suppressed by the nondipole contributions, respectively, if the scatterer points to the forward or backward direction with respect to the light propagation.

- [1] Ph. V. Demekhin *et. al.*, *J. Chem. Phys.* **134**, 024113 (2011).
- [2] R. Dörner *et. al.*, *Phys. Rep.* **330**, 95 (2000).

MO 20.3 Thu 16:30 Empore Lichthof

Measuring discriminatory optical forces on chiral molecules — ●TIANYU FANG, NICK VOGLEY, KILIAN SINGER, and DAQING WANG — Institute of Physics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

We aim at a proof-of-principle experimental demonstration of enantiomer separation using optical forces created by a spatially tailored optical field. Chiral molecules with opposite handedness scatter polarized light differently. Consequently, the scattering of a photon exerts a force on the scatterer. This force can be tailored to be enantiomer specific, such that molecules of opposite handedness are pushed to opposite directions. In this poster, we outline an experiment, in which such discriminatory forces will spatially separate enantiomers in a propagating molecular beam.

MO 20.4 Thu 16:30 Empore Lichthof

Information theoretical approach to coupled electron-nuclear wave packet dynamics: Time-dependent differential Shannon

entropies — ●PETER SCHÜRGER and VOLKER ENGEL — Universität Würzburg, Institut für Physikalische und Theoretische Chemie, Emil-Fischer-Str. 42, 97074 Würzburg, Germany

We study differential Shannon entropies determined from position space quantum probability densities in a coupled electron-nuclear system. In calculating electronic and nuclear entropies, one gains information about the localization of the respective particles and also about the correlation between them. For a Born-Oppenheimer (BO) dynamics the correlation decreases at times when the wave packet reaches the classical turning points of its motion. If a strong non-adiabatic coupling is present, leading to a large population transfer between different electronic states, the electronic entropy is approximately constant. Then, the time-dependence of the entropy reflects the information on the nucleus alone, and the correlation is absent. A decomposition of the entropy into contributions from the participating electronic states reveals insight into the state-specific population and nuclear wave packet localization.

MO 20.5 Thu 16:30 Empore Lichthof

Spectroscopy of the (2)¹Σ_u state in Rb₂ — ●DOMINIK DORER¹, SHINSUKE HAZE¹, MARKUS DEISS¹, EBERHARD TIEMANN², and JOHANNES HECKER DENSCHLAG¹ — ¹Institut für Quantenmaterie, Universität Ulm — ²Institut für Quantenoptik, Leipzig Universität Hannover

We report a systematic study of the (2)¹Σ_u electronic state of the rubidium dimer. For this we carried out single-photon photoassociation spectroscopy with an ultracold sample of ground state atoms. Using either a pulsed or a more narrow cw laser we investigated the vibrational and rotational structure for both isotopologues, ⁸⁷Rb and ⁸⁵Rb. From a theoretical analysis including also previously recorded data from other experiments, we got new insights of spin-orbit and rotational interactions for the (2)¹Σ_u state. These results are also of interest for state-selective molecule detection schemes on the basis of resonance-enhanced multiphoton ionization (REMPI) as the (2)¹Σ_u can serve as an appropriate intermediate state.

MO 20.6 Thu 16:30 Empore Lichthof

Spectroscopic Characterization of Aluminum Monofluoride — ●NICOLE WALTER^{2,1}, JOHANNES SEIFERT¹, BOSIS SARTAKOV¹, and GERARD MEIJER¹ — ¹Fritz Haber Institute of the Max Planck Society, Berlin — ²Humboldt University of Berlin

Aluminum monofluoride (AlF) possesses highly favorable properties for laser cooling, both via the A¹Π and a³Π states. Determining efficient pathways between the singlet and the triplet manifold of electronic states will be advantageous for future experiments at ultralow temperatures. The lowest rotational levels of the A¹Π, *v* = 6 and b³Σ⁺, *v* = 5 states of AlF are nearly iso-energetic and interact via spin-orbit coupling. These levels thus have a strongly mixed spin-character and provide a singlet-triplet doorway. We here present a hyperfine resolved spectroscopic study of the A¹Π, *v* = 6 // b³Σ⁺, *v* = 5 perturbed system in a jet-cooled, pulsed molecular beam. From a fit to the observed energies of the hyperfine levels, the fine and hyperfine structure parameters of the coupled states, their relative energies as well as the spin-orbit interaction parameter are determined. The standard deviation of the fit is about 15 MHz. We experimentally determine the radiative lifetimes of selected hyperfine levels by time-delayed ionization, Lamb dip spectroscopy and accurate measurements of the transition lineshapes. The measured lifetimes range between 2 ns and 200 ns, determined by the degree of singlet-triplet mixing for each level.

MO 20.7 Thu 16:30 Empore Lichthof

Photoelectron Spectroscopy of Simple Diamondoids — ●SIMONE STAHL, PARKER CRANDALL, MARKO FÖRSTEL, and OTTO DÖFFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

Diamondoids are a class of aliphatic molecules with cage-like structures and are a bridge between small hydrocarbons and large nanodiamond macromolecules. Extrasolar nanodiamonds have been discovered in carbonaceous chondrites and could account for more than 5% of cosmic and 40% of tertiary carbon in the interstellar medium.¹ Due to similarities between their infrared spectra and the unidentified infrared emission bands of young stars, diamondoids could be

present in these environments.² However, laboratory measurements of the optical properties of diamondoids, particularly of their cations and functionalized variants, remains incomplete and are necessary for astronomical observations. Here, we present the first photoelectron spectra of cyanoadamantane and amantadine. These are compared to newly measured spectra of adamantane, diamantane, and urotropine, with improved resolution and a more thorough assignment of spectral features with the aid of TD-DFT calculations.^{3,4} The effect of functionalization on the ionization potential, as well as the size and shape of the cage structure on the PES spectrum will be discussed.

1. Henning, Th. & Salama, F. *Science* 282, 2204-2210 (1998).
2. Pirali, O. et al. *ApJ* 661, 919-925 (2007).
3. Schmidt, W. *Tetrahedron* 29, 2129-2134 (1973).
4. Rander, T. et al. *J. Chem. Phys.* 138, 024310 (2013).

MO 20.8 Thu 16:30 Empore Lichthof

Analysis of statistical moments – a new technique to find Legendre coefficients in photoelectron distributions with increased precision — ●SIMON RANECKY, SAGNIK DAS, SUDHEENDRAN VASUDEVAN, TONIO ROSEN, HAN-GYEOL LEE, JAYANTA GHOSH, HENDRIKE BRAUN, ARNE SENFTLEBEN, and THOMAS BAUMERT — Uni Kassel, Experimentalphysik III

The ionisation of isotropically aligned molecules with linear or circular polarized light leads to a characteristic distribution of the photoelectrons. The radial part of the distribution relates to the energy of the photons and the ionisation potential of the molecules. The angular part can be described by Legendre polynomials of the order up to twice the number of photons involved in the ionisation [1].

In velocity map imaging, which we use to detect photoelectrons, the 3d electron distribution is projected electrostatically on a phosphorous screen. The right orientation of the spectrometer leads to no information loss in the Abel-projection, but an Abel-inversion like rbases [2] is necessary to find out the distribution of the Legendre coefficients.

As an alternative way to retrieve the Legendre coefficients, the centroid and higher moments of the photoelectron projection can be used. With the calculated moments of single Legendre polynomials, a linear system of equations can be compiled that makes the Legendre coefficients accessible. For simple photoelectron distributions, we will demonstrate smaller uncertainties as compared to rbases.

- [1] Yang, *Phys. Rev.* 74, 764; Dixit et al., *J. Chem. Phys.* 82, 3546
- [2] Hickstein et al., *Rev. Sci. Instrum.* 90, 065115

MO 20.9 Thu 16:30 Empore Lichthof

Photoelectron circular dichroism on fenchone: from multiphoton to the tunnel ionization regime using near-infrared femtosecond laser pulses. — ●SUDHEENDRAN VASUDEVAN, HAN-GYEOL LEE, SIMON T. RANECKY, NICOLAS LADDA, TONIO ROSEN, SAGNIK DAS, JAYANTA GHOSH, HENDRIKE BRAUN, ARNE SENFTLEBEN, and THOMAS BAUMERT — Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Photoelectron circular dichroism (PECD) is a pronounced forward/backward asymmetry in the ionization of chiral molecules by circularly polarized light. PECD is dominated by the electric-dipole effect, which gives rise to a larger magnitude of asymmetry as compared to circular dichroism in absorption. In this contribution, we use nearly Fourier-limited near-infrared pulses directly from a titanium sapphire femtosecond laser to excite electronic intermediate states in fenchone molecule via a (3+1+1+1) resonance-enhanced multiphoton ionization (REMPI) scheme. We scanned the intensity of the laser and measured the angular distribution of the photoelectrons from the multiphoton almost to the tunnel ionization regime. Herein we present our measured photoelectron spectra, PECD, and mass spectra during the intensity scan.

MO 20.10 Thu 16:30 Empore Lichthof

Temperature-dependant Luminescence and Step-scan FTIR Investigations of Tetranuclear Cu(I) Complexes — ●SOPHIE STEIGER¹, PIT BODEN¹, JASMIN BUSCH², DANIEL MARHÖFER¹, STEFAN BRÄSE², and GEREON NIEDNER-SCHATTEBURG¹ — ¹Department of Chemistry, TUK, Germany — ²IOC, KIT, Germany

In this contribution, we present the investigation of the temperature-dependent luminescence and the luminescent states of tetranuclear copper(I) complexes. The investigations were performed by (time-resolved) luminescence and static as well as step-scan FTIR spectroscopy. The measurements were performed in a temperature range of 290 K to 10 or 5 K in KBr matrix or pure powder. The complexes contain a tetranuclear Cu₄X₄ (X=Cl, Br, I) core and two 2-

(diphenylphosphino)-pyridine ligands with or without a methyl substituent in 4-position of the pyridine ring units. As known from previous work^[1], the same type of complexes with ligands with a methyl group in 6-position shows a pronounced thermochromism, which was not detected for the Cu₄I₄ complex with methyl group in 4-position in KBr matrix. The Cu₄I₄ complex without methyl group shows the thermochromism in powder measurements but it is less resolved in KBr matrix. All other investigated complexes have only slight temperature-dependent shifts in the luminescence. With step-scan FTIR spectroscopy in comparison with quantum chemical calculation, the excited states were assigned to the different excited state structures.

[1] *Chem. Eur. J.* 2021, 27, 5439-5452.

MO 20.11 Thu 16:30 Empore Lichthof

Calculation of the Stark effect of Rydberg states in nitric oxide — ●ALEXANDER TRACHTMANN^{1,4}, FABIAN MUNKES^{1,4}, PATRICK KASPAR^{1,4}, PHILIPP NEUFELD^{1,4}, YANNICK SCHELLANDER^{2,4}, LARS BAUMGÄRTNER^{3,4}, ROBERT LÖW^{1,4}, TILMAN PFAU^{1,4}, and HARALD KÜBLER^{1,4} — ¹⁵. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ²Institut für Großflächige Mikroelektronik, Universität Stuttgart, Allmandring 3b, 70569 Stuttgart — ³Institut für Intelligente Sensorik und Theoretische Elektrotechnik, Universität Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart — ⁴Center for Integrated Quantum Science and Technology (IQST), Universität Stuttgart

We demonstrate Stark effect calculations of high-lying Rydberg states in nitric oxide and compare them to measurements at room temperature. These states are generated using a three-photon continuous-wave excitation scheme. The readout is based on the detection of charged particles created by collisional ionization of Rydberg molecules. Details of the calculation techniques are given.

MO 20.12 Thu 16:30 Empore Lichthof

Decoherence estimates for spin-boson systems from semiclassical Gaussian wavepacket propagation — ●SREEJA LOHO CHOUDHURY¹, CAROLINE LASSER², ROCCO MARTINAZZO^{3,4}, and IRENE BURGHARDT¹ — ¹Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt — ²Technische Universität München, Zentrum Mathematik, Deutschland — ³Department of Chemistry, Università degli Studi di Milano, Italy — ⁴Instituto di Scienze e Tecnologie Molecolari, CNR, Milano, Italy

We investigate the time scale of decoherence in spin-boson type systems, by calculating the subsystem purity as a measure of decoherence. For a general system-bath setting, the decoherence time can be expressed in terms of a universal Gaussian decay of the purity [O. Prezhdo and P. Rossky, *Phys. Rev. Lett.* **81**, 5294 (1998)], but exponential decay is often predicted from Markovian master equations. The transition between these forms of decoherence has recently been discussed [B. Yan and W. H. Zurek, *N. J. Phys.* **24**, 113029 (2022)]. Against this background, we investigate the pure dephasing case in a spin-boson system using semiclassical Gaussian wavepackets, notably relying on the variational multiconfigurational Gaussians (vMCG) [G. A. Worth and I. Burghardt, *Chem. Phys. Lett.* **368**, 502 (2003)] and multiconfiguration time-dependent Hartree (MCTDH) [M. H. Beck, A. Jäckle, G. A. Worth, H.-D. Meyer, *Phys. Rep.* **324**, 1 (2000)] formalism for wavefunction propagation. We further consider quantum-semiclassical hybrid wavefunctions and examine the effect of semiclassical scaling on the subsystem purity.

MO 20.13 Thu 16:30 Empore Lichthof

Photoelectron spectroscopy study of anthracene anions — ●KEVIN SCHWARZ, AGHIGH JALEHDOOST, and BERND V. ISSENDORFF — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

As semiconducting organic materials generate more and more interest, there are still properties of said materials left to be investigated more in depth. After the development of a high temperature-suited pulsed valve to produce clusters of organic material such as anthracene has been concluded recently, first results of energy-resolved photoelectron spectroscopy (PES) studies on anthracene anions (C₁₄H₁₀⁻) are shown.

MO 20.14 Thu 16:30 Empore Lichthof

Action Spectroscopic Infrared Detection of NCCO⁺ — ●MARCEL BAST¹, THOMAS SALOMON¹, OSKAR ASVANY¹, IGOR SAVIĆ², SANDRA BRÜNKEN³, MATHIAS SCHÄFER⁴, STEPHAN SCHLEMMER¹, and SVEN THORWIRTH¹ — ¹I. Physikalisches Institut,

Universität zu Köln, Köln, Germany — ²Department of Physics, Faculty of Sciences, University of Novi Sad, Serbia — ³FELIX Laboratory, Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — ⁴Institute of Organic Chemistry, Department of Chemistry, University of Cologne, Köln, Germany

The linear NCCO⁺ ion has been studied spectroscopically for the first time using the Free Electron Laser for Infrared eXperiments (FELIX) in combination with the 4K 22-pole ion trap facility FELion. The vibrational spectrum of NCCO⁺ was observed in the range from 500 to 1400 and 2000 to 2500 cm⁻¹ using resonant photodissociation of the corresponding Ne-complex. Spectroscopic assignments are in very good agreement with high-level quantum-chemical calculations.

In a consecutive study, the rotationally resolved ν_2 band of the bare NCCO⁺ ion was measured around 2150 cm⁻¹ using the COLTRAP2 instrument in Cologne. Here, the recently developed action spectroscopic method Leak-Out Spectroscopy (LOS)^a was used, that traces the bare ion rather than a weakly bound complex. In this manner, as will be shown on this poster, a nearly background-free absorption spectrum with a large signal-to-noise ratio was obtained.

^a Schmid et al. 2022, J. Phys. Chem. A 126, 43, 8111-8117

MO 20.15 Thu 16:30 Empore Lichthof

Towards probing vibrational dynamics in methyl p-tolyl sulfoxide via time-resolved PECD — ●NICOLAS LADDA, SUDHEENDRAN VASUDEVAN, TONIO ROSEN, HAN-GYEOL LEE, SAGNIK DAS, JAYANTA GHOSH, HENDRIKE BRAUN, ARNE SENFLEBEN, and THOMAS BAUMERT — Institut für Physik, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The goal is to investigate the dynamic change of chiral character upon laser-induced vibrational motion in methyl p-tolyl sulfoxide (MTSO). To this end, we aim to measure the forward/backward asymmetry of the photoelectron angular distribution with respect to the propagation direction of the ionizing circularly polarized light of the randomly oriented chiral molecule, known as photoelectron circular dichroism (PECD) [1]. The vibrational motion - the umbrella motion of the sulfoxide molecule - changes the chiral character of the molecule, which can be investigated by studying the time-resolved PECD with UV femtosecond laser pulses. For this purpose, a two-color pump-probe setup consisting of the 3rd and 4th harmonics of a Ti:Sa laser system is used. The experimental setup has already been tested with static PECD measurements on fenchone and MTSO.

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

MO 20.16 Thu 16:30 Empore Lichthof

Two-photon excitation spectroscopy of metal-organic frameworks — ●HONGXING HAO¹, YANG CUI¹, FERDINAND BERGMEIER², SIMON N. DEGER³, ALEXANDER PÖTHIG³, EBERHARD RIEDLE², ROLAND A. FISCHER³, and JÜRGEN HAUER¹ — ¹Dynamical Spectroscopy, Department of Chemistry, Technical University of Munich, 85748 Garching, Germany — ²Lehrstuhl für BioMolekulare Optik, Ludwig-Maximilians-Universität München, 80538 München, Germany — ³Chair of Inorganic and Metal-Organic Chemistry, Department of Chemistry, Technical University of Munich, 85748 Garching, Germany

Metal-organic frameworks (MOFs) or coordination polymers (CPs) constitute a novel class of materials and have several interesting photo-physical properties such as a high multiphoton absorption cross section. Here, we introduce a spectroscopic experiment to measure two-photon excitation spectra from the visible to the near infrared based on a non-collinear optical parametric amplifier and a phase-stable common-path birefringent interferometer via nonlinear Fourier-transform spectroscopy. We present two-photon excitation spectra in the range between 380 to 470 nm with a data acquisition time of under one minute per spectrum.

We demonstrate the feasibility of this approach by using standard dyes as test samples. After incorporating two-photon absorption active organic linker molecules in crystalline CPs or MOFs, the spectra show a shift of oscillator strength. We suggest excitonic coupling between the linkers as the mechanism behind this targeted modification of two-photon absorption property.

MO 20.17 Thu 16:30 Empore Lichthof

Control of (bio-) nanoparticles with external fields — ●JINGXUAN HE^{1,2,3}, LENA WORBS^{1,2}, JANNIK LÜBKE^{1,2,3}, SURYA KIRAN PERAVALI^{1,4}, ARMANDO D. ESTILLORE¹, AMIT K. SAMANTA^{1,3}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Department of Physics, Universität Hamburg, Germany — ³Center for Ultrafast Imaging, Universität Hamburg, Germany — ⁴Fakultät für Maschinenbau, Helmut-Schmidt-Universität, Germany

Unraveling the elementary steps of biological processes and chemical reactions is a long-time goal of the scientific community. By using x-ray single-particle diffractive imaging, we can investigate the three-dimensional molecular structure of individual nanoparticles at atomic resolution through reconstructing a series of two-dimensional diffraction patterns [1]. However, because of the typically low signal-to-noise ratio, this requires the collection of a large amount of individual diffraction patterns. Since every intercepted particle is destroyed by the intense x-ray pulse, a new and preferably identical sample particle has to be delivered to every pulse. Here, we present an approach to prepare dense beams of cold and controlled nanoparticles and macromolecules with buffer-gas-cell-cooling and aerodynamic-focusing techniques. Besides, we demonstrated several control mechanisms with external fields that can help to realize a stream of pure, identical particles. We also showed that the particles' arbitrary orientation in space can be controlled by applying laser alignment.

[1] M. M. Seibert, et al., *Nature* **470**, 78 (2011)

MO 20.18 Thu 16:30 Empore Lichthof

TrapREMI: A reaction microscope inside an electrostatic ion beam trap — FRANS SCHOTSCH¹, ●ILJA ZEBERGS¹, SVEN AUGUSTIN^{1,2}, HANNES LINDENBLATT¹, LUDWIG HOIBL³, DENIS DJENDJUR³, CLAUDIUS DIETER SCHRÖTER¹, THOMAS PFEIFER¹, and ROBERT MOSHAMMER¹ — ¹Max-Planck-Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Baden-Württemberg, Germany — ²Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen, Switzerland — ³Department of Physics and Astronomy, Ruprecht-Karls University, 69120 Heidelberg, Baden-Württemberg, Germany

A novel setup has been developed to investigate the reaction dynamics of (molecular) ions with a variety of projectiles in kinematically complete crossed-beam experiments. The setup combines an electrostatic ion beam trap (EIBT) with a reaction microscope (REMI).

The EIBT stores ions in oscillatory motion at several keV and allows further preparation e.g. cooling, relaxation, pulsing of the beam, mass selection. Reactions are induced by crossing the ion beam with another beam in the field-free region of the EIBT, where the REMI is located. The REMI, oriented along the target beam axis, allows for detection of all fragments in coincidence, including neutral particles, and reconstruction of their 3D-momenta.

During first REMI tests a laser pulse was used as the projectile to induce photodissociation in molecular ions. Currently a gas jet was assembled to provide an atomic/molecular beam and first simple ion-atom/molecule collision experiments are conducted.

MO 20.19 Thu 16:30 Empore Lichthof

Collisional excitation and dissociation of CO molecules by ion impacts and applications to astrophysics — ●MASATO NAKAMURA — College of Science and Technology, Nihon University, Funabashi, Japan

The CO molecule is one of the most abundant molecules in interstellar space and a major component of the stellar (solar) winds is proton. Thus, the collisional excitation and collision-induced dissociation (CID) by proton impacts are expected to play important roles in the chemical evolution of interstellar molecules. Here we present a theoretical work on the energy transfer and fragmentation of CO molecule by proton impact at hyperthermal energies. The classical trajectory calculation and the sudden-limit model are applied to estimate the energy transfer from translational to internal degrees of freedom. The threshold energy for the dissociation is calculated by for the impact of singly charged ions. For comparison, the calculation is performed also for nitrogen molecule. The nitrogen molecule is a major component of atmosphere of Titan.