

MO 12: Posters 2: Molecular Dynamics, Clusters, and High Resolution Spectroscopy

Time: Wednesday 17:00–19:00

Location: P OGs

MO 12.1 Wed 17:00 P OGs

Photoionization of Ne_2 : localized or delocalized? — HENDRIK SANN¹, ●ABIR MHAMDI², FLORIAN TRINTER¹, MARKUS SCHÖFFLER¹, PHILIPP V. DEMEKHIN², TILL JAHNKE¹, and REINHARD DÖRNER¹ — ¹Institut für Kernphysik, Universität Frankfurt, Frankfurt am Main, Germany — ²Institut für Physik, Universität Kassel, Kassel, Germany

We provide conclusive experimental evidence that for the van der Waals dimer Ne_2 , a proper post-selection of photoelectrons yields electron angular distributions which are of well-defined parity [1]. This post-selection can be achieved for $2p$ -ionization by detecting the fragmentation of the Ne_2^+ into $Ne^+ + Ne$, and it is possible because the potential energy curve $2\Sigma_g^+$ is the only dissociating state of $Ne_2^+(2p^{-1})$. The electron angular distribution for this dissociative state, measured by the COLTRIMS [2] technique, is symmetric with respect to the direction to which the charged fragment is emitted. The present observations are supported by ab-initio electronic structure and dynamics calculations which were carried out by the Single Center method and code [3]. We conclude that the picture of localization or delocalization of a single particle or hole in this many-body wave function is oversimplified. In coincidence experiments on molecular ionization, one has to carefully discuss what is veritably measured and to which basis this measurement projects set the few-body wave function just as in any coincidence measurement on entangled photons.

References: [1] H. Sann, et al., *Phys. Rev. Lett.*, in press (2016). [2] R. Dörner, et al., *Physics Reports* **330**, 96 (2000). [3] Ph. V. Demekhin, et al., *Journal of Chemical Physics* **134**, 024113 (2011).

MO 12.2 Wed 17:00 P OGs

Collective resonances in dilute vapors — ●LUKAS BRUDER, ULRICH BANGERT, MARCEL BINZ, and FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg

We have developed a phase-modulated pump-probe method which allows for efficient isolation and detection of multiple-quantum coherence signals. With this, we observed for the first time higher-order collective resonances in dilute atomic vapors [1]. The origin of these signals is debated since interatomic interactions are small in these systems [2]. Recently, we have significantly improved the spectral resolution in our setup (~ 1 GHz) and characterized the phase signature of the observed resonances. This revealed a phase characteristic depending on the fundamental hyperfine states. Our results have triggered interest from several theory groups currently working on an explanation of this phenomenon.

[1] L. Bruder, M. Binz, and F. Stienkemeier, *Phys. Rev. A* **92**, 053412 (2015).

[2] S. Mukamel, *J. Chem. Phys.* **145**, 41102 (2016).

MO 12.3 Wed 17:00 P OGs

A Velocity Map Imaging setup to benchmark technologies enabling the study of new systems on ion-molecule reactions — ●PATRICK STRÜBIN, FRANZISKA KRAMMER, TIM MICHAELSEN, JENNIFER MEYER, ATILAY AYASLI, BJÖRN BASTIAN, and ROLAND WESTER — Institut für Ionen und Angewandte Physik, Universität Innsbruck, Austria

Our group studies the dynamics of ion-molecule reactions by crossed-beam Velocity Map Imaging (VMI) [1]. For neutral reactions there have been a lot of investigations on the influence of excited vibrational states prior to the reaction [2]. We are planning to extend this research to ion-molecule reactions. As a first step a new crossed-beam VMI setup has been built. It will be used for measurements to determine the fraction of molecular excitation in the neutral molecular beam by a tunable optical parametric oscillator laser.

Furthermore we will extend our research to metal ion reactions with hydrocarbons. To produce metal ions we will use a laser vaporisation source [3,4] attached to the VMI spectrometer. Here we present test measurements and design considerations for the new VMI spectrometer, the metal ion source and the laser excitation scheme.

[1] R. Wester, *Phys. Chem. Chem. Phys.* **16**, 396 (2014)

[2] K. Liu, *J. Chem. Phys.* **142**, 080901 (2015)

[3] T. G. Dietz et al., *J. Chem. Phys.* **74**, 6511 (1981)

[4] D. Proch and T. Trickl, *Rev. Sci. Instrum.* **60**, 713 (1989)

MO 12.4 Wed 17:00 P OGs

Coinage bimetallic complexes display ultrafast multiexponential electronic dynamics in an ion trap and in solution — ●FLORIAN BÄPPLER¹, SEBASTIAN KRUPPA², YEVGENIY NOSENKO², ROLF DILLER¹, and CHRISTOPH RIEHN^{2,3} — ¹Department of Physics — ²Department of Chemistry, TU Kaiserslautern — ³Forschungszentrum OPTIMAS, 67655 Kaiserslautern

Bimetallic coinage metal complexes of type $[Me_2(dcpm)_2]^{2+}$, 1^{2+} , (Me= Ag, Au; dcpm = bis(dicyclohexylphosphino)methane) are stabilized by metal-metal interactions and give rise to interesting optical properties for OLEDs, photocatalysis, and sensory applications. Their excited state dynamics have been investigated in parallel in gas phase by femtosecond photo-induced dissociation and in solution by transient absorption. Both studies report a multiexponential electronic decay after excitation of metal-centered states modulated by solvent molecules and counter ions.

MO 12.5 Wed 17:00 P OGs

Collinear Phase-modulated Femtosecond Pump-Probe Experiments Using a Low Repetition-rate Laser System — ●MARCEL BINZ, LUKAS BRUDER, ULRICH BANGERT, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

A particularly robust and very versatile stabilization method for coherent time-resolved spectroscopy is the phase-modulation approach [1], [2]. The combination of continuous acousto-optical phase-modulation with lock-in detection greatly improves the signal-to-noise ratio and the sensitivity in this scheme. However, the method was thought to be suitable only for high repetition-rate laser systems ($\gtrsim 200$ kHz) which are not available in many labs.

Recently, we have successfully implemented this technique in a pump-probe scheme with fs laser pulses at 5 kHz repetition-rate. We found that much higher modulation frequencies than laser repetition-rates can be used without losing performance. This effect, which we call phase-synchronous undersampling, shows promise for the implementation of the phase-modulation scheme in even lower repetition-rate XUV laser sources by shifting the carrier frequency far away from the low frequency noise spectrum.

[1] P. F. Tekavec, T. R. Dyke, and A. H. Marcus, *J. Chem. Phys.* **125**, 194303 (2006).

[2] L. Bruder, M. Mudrich, and F. Stienkemeier, *Phys. Chem. Chem. Phys.* **17**, 23877 (2015).

MO 12.6 Wed 17:00 P OGs

Time-resolved XUV photoelectron spectroscopy of organic dyes in solution — ●JOHAN HUMMERT, IVGENII INKONNIKOV, NICOLA MAYER, MARTIN ECKSTEIN, and OLEG KORNILOV — Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin

The electronic dynamics of organic molecules after photoexcitation are of great interest for biologically relevant systems as well as synthetic functional complexes. Often the environment, in many cases an aqueous solution, has a strong influence on the electronic structure. With the development of the liquid jet technique [1] methods demanding high vacuum conditions became applicable to molecules in solution.

The method employed here is time-resolved XUV photoelectron spectroscopy. Wavelength-selected high harmonics provided by a recently developed monochromator setup [2] are applied to probe the electronic relaxation of solvated molecules after single photon excitation with visible light. The high collection efficiency of a magnetic bottle spectrometer enables us to clearly distinguish molecular signals from strong solvent signals.

In a benchmark experiment with the water soluble dye "Quinoline Yellow WS" we measure ground state ionization energies and observe relaxation of excited states in solution. Excited state spectra and decay constants can be measured for concentrations down to 10 mM, which establishes this technique for a wide range of samples.

[1] Faubel et. al., *J. Chem. Phys.* **106**, 9013-31 (1997)

[2] Eckstein et. al., *JPCL* **6**, 419-25 (2015)

MO 12.7 Wed 17:00 P OGs

Exploring Non-local Autoionization in Water Clusters and Aqueous Solutions — ●CLEMENS RICHTER¹, MARVIN N. POHL², CLARA SAAK⁴, MELANIE MUCKE⁴, EVGENY LUGOVOY¹, ROBERT

SEIDEL², EMAD F. AZIZ², BERND ABEL¹, BERND WINTER², and UWE HERGENHAHN^{1,3} — ¹Leibniz Institute of Surface Modification, Leibzig, Germany — ²Helmholtz-Zentrum Berlin, Berlin, Germany — ³Max-Planck-Institut für Plasmaphysik, Greifswald, Germany — ⁴Uppsala University, Uppsala, Sweden

Interaction of matter with ionizing radiation leads to emission of a multitude of electrons, either by direct photoemission or via secondary pathways, i.e. local and non-local autoionization. While the local Auger process is well established, the non-local processes intermolecular coulombic decay (ICD) and electron transfer mediated decay (ETMD) are topics of current research. Since both processes lead to the emission of low energy electrons - a primary source of radiation damage - we investigate autoionization in water and aqueous solutions of biological relevance. In our experiments electron-electron coincidence spectroscopy is performed using a magnetic bottle electron spectrometer. We present two examples of our current research on water-uracil clusters applying our newly constructed source for solvated biomolecule clusters as well as our first coincidence measurements of Li salt solutions using a liquid jet. While in the water-uracil clusters ICD is the predominant autoionization process. The Li salt solutions unambiguously display an ETMD signature. Moreover, we discuss ETMD spectroscopy as potential tool for measuring contact ion pairs in solution.

MO 12.8 Wed 17:00 P OGs

Fluorescence dynamics and quantum yield measurements of a polycyclic tetrazolium compound in dependence on solvent viscosity — •JAN-LUCAS WREE, TOM BOLZE, and PATRICK NUERNBERGER — Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum

The color change of tetrazolium salts that occurs during enzymatic reduction to formazans is exploited in applications like monitoring cell growth, since it can be conveniently measured in a quantitative fashion. Some particular tetrazolium compounds are known to further exhibit fluorescence, like the phenyl-benzo[c]tetrazolo-cinnolinium (PTC) which is investigated in this contribution.

We explore the fluorescence properties of PTC in alcoholic solvents whose viscosity span several orders of magnitude. Static measurements of absorption and fluorescence characteristics as well as of fluorescence quantum yields, measured against several reference compounds, are compared to the excited-state lifetimes obtained from time-correlated single-photon counting (TCSPC). The studies disclose that the emission characteristics vary but do not drastically change with solvent viscosity. This indicates that the emitting state is also deactivated by a competing, non-radiating reaction channel, but not by one that involves large intramolecular rotational motion, a process that would be strongly slowed down in more viscous solvents, as found for instance in molecular rotors or ultrafast C=C photoisomerization.

MO 12.9 Wed 17:00 P OGs

IR & UV/Vis spectroscopic studies on a luminescent heteroleptic mononuclear copper(I)-complex — •MERTEN GRUPE¹, FABIAN DIETRICH², STEFAN BRÄSE³, MARKUS GERHARDS², and ROLF DILLER¹ — ¹Dept. of Physics, TU Kaiserslautern, 67663 Kaiserslautern — ²Dept. of Chem., TU Kaiserslautern, 67663 Kaiserslautern — ³Dept. of Org. Chem., KIT, 76131 Karlsruhe

Luminescence in copper-complexes is controlled by several photoinduced intra- and intermolecular processes, such as molecular flattening, intersystem crossing, solvation etc. For the elucidation of the underlying photophysics we employed femtosecond IR & UV/Vis transient absorption (TA) as well as transient anisotropy measurements and DFT calculations on a highly efficient luminescent heteroleptic mononuclear [1] copper(I)-complex. The results allow a rigorous comparison of the ultrafast dynamics in the UV/Vis spectral region with literature reports [2] [3] [4] on homoleptic copper(I)-complexes. Femtosecond IR TA facilitates an extended specification of the ultrafast processes in the heteroleptic mononuclear [1] copper(I)-complex.

[1] L. Bergmann et al. Chem. Commun., 2013, 49 6501

[2] M. Iwamura et al. Acc. Chem. Res., 2015, 48, 782-791

[3] G. B. Shaw et al. J. Am. Chem. Soc., 2007, 129, 2147-2160

[4] Z. A. Siddique et al. Inorganic Chemistry, 2003, 42, 6366-6378.

MO 12.10 Wed 17:00 P OGs

Photophysics of porphyrin-based surface-anchored metal-organic frameworks investigated by time-resolved optical and EPR spectroscopy — •MICHAEL ADAMS¹, ROWAN W. MACQUEEN², MICHAEL OLDENBURG¹, JAN BEHREND³, KLAUS

LIPS², BRYCE S. RICHARDS¹, and IAN A. HOWARD¹ — ¹Institute of Microstructure Technology, Karlsruhe Institute of Technology — ²Berlin Joint EPR Lab, Helmholtz-Zentrum Berlin für Materialien und Energie — ³Berlin Joint EPR Lab, Fachbereich Physik, Freie Universität Berlin

Surface Anchored Metal Organic Frameworks (SURMOFs) are hybrid materials comprised of crystalline networks of organic molecules linking metal centers. The organic linkers may be active chromophores, and the structural order of the molecular assembly can give rise to intriguing new effects that differ from those observed in the lone chromophores. SURMOFs whose linkers are based on porphyrin chromophores have already stimulated interest due to their exhibition of photovoltaic action, and their ability to generate and transport triplet excitonic states to enable triplet-triplet annihilation upconversion. However, many fundamental questions regarding the photophysics of this system remain. In this contribution we provide a deeper insight into the SURMOF-2 structure using palladium porphyrin linkers by combining transient absorption spectroscopy (TAS), time-dependent luminescence and transient electron paramagnetic resonance (TEPR) measurements in order to elucidate the formation and transition between triplet, triplet aggregate, and radical species following photoexcitation.

MO 12.11 Wed 17:00 P OGs

Frequency conversion of organotetrelchalcogenide clusters — •NILS W. ROSEMAN¹, JENS P. EUSSNER², EIKE DORNSIEPEN², STEFANIE DEHNEN², and SANGAM CHATTERJEE¹ — ¹Institute of Experimental Physics I, Justus-Liebig-Universität Giessen, Heinrich-Buff Ring 16, D-35392 Giessen, Germany — ²Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35043 Marburg, Germany

Cluster molecules based on organotin complexes do feature versatile properties. One of which is low-threshold nonlinear white-light generation [1]. This process is tentatively being assigned to the driven motion of delocalised electrons in the clusters ground state potential. To review this explanation, a systematic variation of the cluster components and correlation to the nonlinear response is crucial. Here, we present to nonlinear optical response of a series of organotetrelchalcogenide clusters based on the compound presented in [1]. Variation of the delocalised electron system is performed by changing the ligands, while the fundamental optical transition is changed by variation of the tetrel-moiety. Resulting in a drastic change of the nonlinear response; from white-light to second harmonic generation. [1] N. W. Rosemann et al., *A Highly Efficient Directional Molecular White-Light Emitter Driven by a Continuous-Wave Laser Diode*, Science **352**, 1301-1304 (2016)

MO 12.12 Wed 17:00 P OGs

Probing the anisotropic electronic structure of silicon cluster cations — •MARKO FÖRSTEL, BERTRAM JAEGER, PHILIPP SPORKHORST, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Silicon is among the ten most abundant elements in our universe. In its ionic form it was found in the interstellar medium and even in the Earth's atmosphere. The Si⁺ ion also plays a role in manufacturing processes of silicon based semiconductors. Here we set out to study the hitherto poorly understood fundamental chemistry and behavior of Si_n⁺ ions. A recently updated tandem mass spectrometer coupled with a laser vaporization source [1] is utilized to study the molecular structure of Si_n⁺-Ar_m cluster ions. Depending on cluster source conditions, we observe magic numbers in these systems that indicate structures which are strongly influenced by the anisotropic electron density of the central Si_n⁺ ion. We describe the updated setup, present the experimental mass spectra and discuss the possible cluster structures underlying these magic numbers. Our discussion is supported by quantum chemical calculations.

[1] Photodissociation spectrum and structure of Au₄⁺-H₂O clusters, Jaeger, B. K. A., Savoca, M., Dopfer, O., and Truong, N. X., International Journal of Mass Spectrometry (402) 2016.

MO 12.13 Wed 17:00 P OGs

XRD/SEM/EDX characterization of green synthesized silver nanoparticles — MIROSLAV CVETINOV¹, MAJA STOJANOVIC¹, MILOŠ BOKOROV¹, SLOBODAN GLISIC², and •MILORAD ČAKIC² — ¹Faculty of Science, University of Novi Sad, Trg Dositeja Obradovica

4, Novi Sad, Serbia — ²Faculty of Technology, University of Nis, Bulevar Oslobođenja 124, Leskovac, Serbia

Due to the fact that silver nanoparticles (AgNP) exhibit broad spectrum of biocidal activity, they are often employed in industrial and consumer goods sectors. For the purpose of synthesis of green AgNPs, we used aqueous extract of *Fumaria officinalis* (earth smoke) obtained in alkaline solution resting for 5 days at room temperature (RT) as well as resting for 2 hours on boiling temperature of the reaction mixture (BT). Newly synthesized specimens were investigated by the methods of X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). XRD confirmed crystallization of AgNP in face-centred cubic lattice (space group Fm-3m, lattice constant $a = 4.086 \text{ \AA}$). Using Scherrer equation on the most intense Ag peak in XRD spectra at Bragg angle $2\theta = 38.1^\circ$ we obtained average nanoparticle size of 21nm and 18nm for the RT and BT synthesized specimens, respectively. At specific points on specimen surface, EDX showed maximum Ag concentration of 44% and 81% for RT and BT synthesized specimens, respectively. This study presents convenient way to synthesize silver nanoparticles using plant materials. AgNPs obtained by this method show promising potential in drug formulations production as well as in biomedical and agricultural applications.

MO 12.14 Wed 17:00 P OGS

Cryogenic Matrix Isolation FTIR Spectroscopy with Diamond Beam Splitter. — ●DMITRY STRELNİKOV¹, BASTIAN KERN², CHRISTOPH SÜRGER³, and MANFRED KAPPE¹ — ¹Physikalische Chemie, KIT, Karlsruhe, Germany — ²MPI for Solid State Research, Stuttgart, Germany — ³Physikalisches Institut, KIT, Karlsruhe, Germany

FTIR spectroscopy is a robust technique to obtain broad band spectra of various species. In case of valuable samples, which can be kept only at cryogenic temperatures and require long preparation time, one would like to measure in all accessible spectral regions. To extend the spectroscopic measurement range from Far-IR to near-IR a synthetic diamond beam splitter without compensator plate and UHV diamond viewports were installed in a Bruker IFS66v/S FTIR spectrometer. We have also modified the IR detector chamber to allow measurements with 5 different detectors. We demonstrate performance of the upgraded FTIR spectrometer by presenting measurements of matrix isolated fullerene ions and an adhesive tape.

MO 12.15 Wed 17:00 P OGS

IR spectroscopy of cationic nickel ethanol clusters - variation of cluster size and solvation shell — ●DANIEL BELLAIRE, MARKUS BECHERER, FABIAN DIETRICH, and MARKUS GERHARDS — TU Kaiserslautern, Fachbereich Chemie and research center OPTIMAS, Erwin-Schroedinger-Straße 52, 67663 Kaiserslautern

Clusters containing transition metals and aliphatic ligands provide model systems regarding e.g. catalytic properties, magnetism, reactivity and structure. Furthermore, investigation of clusters may reveal potential cooperative effects. Thus, the successive variation of size and ligand number of the metal clusters can give a fundamental insight. The investigated nickel clusters are produced by applying laser ablation to a rotating metal rod and by attaching the ethanol ligand(s) in a supersonic beam. The frequencies and frequency shifts of OH stretching vibrations (between different clusters) are probed by means of IR-photofragmentation spectroscopy. An assignment of structure and spin states is performed by comparing the experimentally observed vibrational frequencies with the calculated values obtained from DFT calculations.

Specifically, cationic $\text{Ni}_m(\text{ethanol})_n^+$ ($m=2-4$; $n=1-3$) clusters are spectroscopically investigated and explored by the aforementioned methods. The results give insight both into the structure and reactivity of the nickel aggregates.

MO 12.16 Wed 17:00 P OGS

High resolution spectroscopy on KCa — ●JULIA GERSCHMANN¹, ERIK SCHWANKE¹, HORST KNÖCKEL¹, SILKE OSPELKAUS¹, ASEN PASHOV², and EBERHARD TIEMANN¹ — ¹QUEST und Inst. f. Quantenoptik, Leibniz Universität Hannover — ²Sofia Universität "St. Kliment Ohridski", Bulgarien

The mixed alkali-alkaline earth molecules have recently attracted the interest of the scientific community due to possible applications in the field of cold and ultracold molecules. The combination of an alkaline and an alkaline earth atom leads to molecules which have permanent electric and magnetic dipole moments and thus offer manipulation of

their states by external fields. Several ab initio calculations have been published on various combinations of a group IA and a group IIA atom from which one expects $2\Sigma^+ - 2\Sigma^+$ transitions in the near infrared. Experimentally, not so much is known about the molecular electronic states. The KCa molecules were created in a heatpipe oven and their thermal emission was recorded via a high resolution Fourier transform spectrometer. We have used laser induced fluorescence to assign the vibrational band heads of transitions from $v' \leq 2$ to $v'' \leq 3$ in the $2^2\Sigma^+ - 1^2\Sigma^+$ system. The resulting vibrational constants predicted other, moderately higher bandheads which can be observed in the emission spectrum. We are able to describe the rovibrational spectrum up to $N = 160$ of the $v = 0$ and $v = 1$ levels of the ground state of KCa. The rovibrational spectrum can be described by a Dunham series and one coefficient for the spin-rotation coupling. We will report on the status of the investigations.

MO 12.17 Wed 17:00 P OGS

High-resolution spectroscopy on the hyperfine structure of small aluminum-bearing molecules and analysis of their resulting electronic structures — ●BJÖRN WASSMUTH¹, ALEXANDER BREIER¹, GUIDO W. FUCHS¹, THOMAS F. GIESEN¹, and JÜRGEN GAUSS² — ¹Institute of Physics, University of Kassel, 34132 Kassel, Germany — ²Institute of Physical Chemistry, University of Mainz, 55099 Mainz, Germany

We investigate metal-containing small molecules in the gas phase by means of millimeter/submillimeter-wave spectroscopy. The experimental investigation is guided by high-level quantum chemical calculations performed at Mainz.

Al^{16}O , Al^{32}S , and Al^{34}S are produced by laser ablation of solid aluminum and a dilution of N_2O (2%) or H_2S (7%) in helium buffer gas, that subsequently undergoes an adiabatic expansion in our vacuum chamber. The resulting molecular beam is probed by monochromatic radiation in the frequency range up to 400 GHz. Measurements reveal the hyperfine structure of these linear molecules to follow Hund's case $b_{\beta S}$ coupling due to the nuclear spin of aluminum.

From the rotational constants the bond lengths are obtained. Analysis of our data including the hyperfine parameters of AlX (with $X \in \{\text{F}, \text{Cl}, \text{Br}, \text{I}\}$) reveals details of the respective electronic structures. With the present work new molecular parameters for future measurements on AlY (with $Y \in \{\text{N}, \text{P}\}$) are predicted.

MO 12.18 Wed 17:00 P OGS

Infrared spectroscopic investigations of N_2 adsorbed to cold Rhodium Iron alloy cluster cations — ●MATTHIAS KLEIN, AMELIE EHRHARD, SEBASTIAN DILLINGER, JENNIFER MOHRBACH, and GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie und Forschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

We investigated the N_2 adsorption behavior of bimetallic Rhodium-Iron cluster cations ($[\text{Rh}_l\text{Fe}_m(\text{N}_2)_m]^+$), $l = n = 3 - 8$ and $m = 1 - 10$, and their geometric structures by means of InfraRed PhotoDissociation (IRPD) spectroscopy in comparison with DFT modelling. For $l = n = 3$ and 4 DFT suggests alloy structures, in case of $l = n = 4$ of high (D_{2d}) symmetry: N_2 adsorption and IRPD studies find strong evidence for preferential adsorption to Rh sites and mere secondary adsorption to Fe. The spectroscopic findings are well interpreted for the smaller clusters in terms of the computed structures, while the many details in the spectra of the larger clusters are subject of ongoing work.

MO 12.19 Wed 17:00 P OGS

Combined IR/UV investigations on isolated peptides: structural assignments for cyclic tetrapeptides — ANKE STAMM¹, ●DOMINIQUE MAUÉ¹, KIRSTEN SCHWING¹, ASTRID SCHALY², STEFFEN SCHLICHER², JULIA BARTL², STEFAN KUBIK², and MARKUS GERHARDS¹ — ¹TU Kaiserslautern, Dept. of Chemistry, Physical Chem. — ²TU Kaiserslautern, Dept. of Chemistry, Organic Chem., Erwin-Schrödinger-Str. 52/54, 67663 Kaiserslautern

Cyclopeptides are a widespread class of substances in nature with the antibiotic valinomycin being one of the most famous representatives. Their physiological effects are frequently based on the tendency to form bioactive conformations. Therefore the investigation of their structure is of great importance for understanding their functionalities. The mass- and isomer-selective combined IR/UV spectroscopy in molecular beam experiments represents a powerful tool for the structural investigation on isolated molecules in the gas phase. In combination with DFT calculations we are able to perform structural assignments for the

electronic ground state. Here we present a structural determination for three different cyclic tetrapeptides, cyclo[L-Tyr(Me)-D-Pro-L-**R**-D-Pro] (**R**= Tyr(Me), Ala, Glu(Me)). A structural assignment with two intramolecular hydrogen bonds can be observed. Due to the asymmetric subunits there are different binding motifs within the cyclic tetrapeptide with R=Ala, Glu(Me) possible.

MO 12:20 Wed 17:00 P OGs

High resolution spectroscopy on LiSr — •ERIK SCHWANKE, JULIA GERSCHMANN, HORST KNÖCKEL, SILKE OSPELKAUS, and EBERHARD TIEMANN — QUEST und Inst. f. Quantenoptik, Leibniz Universität Hannover

The mixed alkali-alkaline earth molecules have recently attracted the interest of the scientific community due to possible applications in the field of cold molecules. These molecules have permanent electric and magnetic dipole moments and thus offer manipulation of their states

by external fields. Several ab initio calculations have been published for LiSr from which one expects $^2\Sigma^+ - ^2\Sigma^+$ transitions in the near infrared. We have successfully recorded the near infrared spectrum of LiSr in a heatpipe oven. The thermal emission was recorded via a high resolution Fourier transform spectrometer. The assignment of the spectrum was facilitated by tuning a diode laser to an emission line, resulting in the observation of P-R-doublets and a simple vibrational progression in the fluorescence. Rotational constants from ab initio-calculations were used for a first guess of the rotational quantum numbers. Then we proceeded to take into account more transitions from higher rotational and vibrational levels. We are able to describe the rovibrational spectrum for the lowest vibrational states, deriving molecular parameters for the ground state $1^2\Sigma^+$. Perturbations due to couplings between the $2^2\Sigma^+$ state and the $1^2\Pi$ state have been observed and are used to investigate the $^2\Sigma_{1/2}^+ - 1^2\Pi_{1/2}$ and $^2\Sigma_{1/2}^+ - 1^2\Pi_{3/2}$ couplings. We will report on the status of the investigations.