MO 22 Poster I

Zeit: Samstag 10:30–12:30 Raum: Poster HU

MO 22.1 Sa 10:30 Poster HU

Spectroscopic studies of the NaCs triplet ground state — •H. Knöckel[1], O. Docenko[2], E. Zaharova[2], M. Tamanis[2], R. Ferber[2], A. Pashov[3], and E. Tiemann[1] — [1]Institut für Quantenoptik, Universität Hannover — [2]Department of Physics and Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia — [3]Institute for Scientific Research in Telecommunications, Sofia, Bulgaria

Recent success in the photoassociation of heteroalkalis, like RbCs [1] and KRb [2], demands for detailed spectroscopic studies, especially close to the atomic asymptote, to get better predictions for further experiments. The ground state $X^1\Sigma^+$ of NaCs has been recently studied by laser induced fluorescence Fourier-transform spectroscopy [3]. Here we present the studies of the first triplet state $a^3\Sigma^+$ in NaCs.

The state $a^3\Sigma^+$ was studied by high resolution Fourier transform spectroscopy. Transitions to the triplet manifold with partially resolved hyperfine structure were observed by exciting the strongly mixed $B^1\Pi$ - $c^3\Sigma^+$ - $b^3\Pi$ system. The analysis of the long-range potential energy curves related to the atomic 3s(Na)+6s(Cs) asymptote provides important information for description of the interaction between a Na and a Cs atom in their ground states at low kinetic energies, thus cold temperatures. The present status of the investigation will be reported. The work is supported by DFG through SFB 407. O.D., M.T. and R.F. acknowledge the support by a NATO grant and by the EC 5th Frame Growth Grant.

[1] A.J. Kerman et al., Phys. Rev. Lett. 92, 033004 (2004)

[2] D. Wang et al., Phys. Rev. Lett., in print (arXiv:physics/0410220)

[3] O. Docenko et al., Eur. Phys. J D, in print

MO 22.2 Sa 10:30 Poster HU

Interactions between K (4^2S) and Rb (5^2S) on the triplet potential surface — •H. Knöckel[1], O. Docenko[2], E. Zaharova[2], M. Tamanis[2], R. Ferber[2], A. Pashov[3], and E. Tiemann[1] — [1]Institut für Quantenoptik, Universität Hannover — [2]Department of Physics and Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia — [3]Institute for Scientific Research in Telecommunications, Sofia, Bulgaria

Molecular spectroscopy has proven to offer powerful tools for investigating interactions between atoms at short as well as at long internuclear distances (e.g. [1]). Precise and abundant experimental data led to accurate characterization of potential energy surfaces in a variety of atom pairs [2]. This present contribution focuses on the interaction between K and Rb atoms in their ground state on the triplet surface $a^3\Sigma^+$. This atomic pair attracted recently significant attention in the context of ultracold heteronuclear collisions and formation of translationally cold polar molecules and molecular Bose-Einstein condensates (e.g. [3,4]). New experimental data were obtained by means of high resolution Fourier transform spectroscopy. The present status report of the research will include analysis of the partially resolved hyperfine structure of the transitions and first estimates on the shape of the potential energy curve. The work is supported by DFG through SFB 407. O.D., M.T. and R.F. acknowledge a NATO grant and the EC 5th Frame Growth Grant. [1] C. Samuelis et al. Phys. Rev. A 63, 012710 (2001) [2] O. Docenko et al. Phys. Rev. A 69, 042503 (2004) [3] D. Wang et al. , arXiv:physics/0410220 [4] J. Goldwin et al. Phys. Rev. A 70, 021601 (2004)

MO 22.3 Sa 10:30 Poster HU

Stark-Abbremsung und Kühlung von großen Molekülen — •Jochen Küpper, Kirstin Wohlfart, Henrik Haak und Gerard Meijer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

Die Untersuchung von Biomolekülen in der Gasphase ist ein wichtiger Ansatz zu einem detaillierten Verständnis der *Bausteine des Lebens*. In den letzten Jahren wurden große Fortschritte bei der Untersuchung der intrinsischen Eigenschaften von Biomolekülen mit Hilfe von Gasphasenspektroskopie gemacht [1,2]. Die Erzeugung ultrakalter, isolierter Biomoleküle erlaubt weitergehende Untersuchungen mittels hochauflösender Spektroskopie und Streuexperimenten. In unserer Arbeitsgruppe haben wir Methoden entwickelt, um neutrale, polare Moleküle mit Hilfe zeitlich variierender hoher elektrischer Felder abzubremsen und zu kühlen [3]. Hier demonstrieren wir, wie diese Methoden auf große organische und biologisch relevante Moleküle übertragen werden können. Wir haben ein neues Experiment zur Abbremsung von Molekülen in hochfeldsuchenden Zuständen aufgebaut. Hier stellen wir erste Ergebnisse zur Fokussierung und Abbremsung vor und diskutieren weitergehende Experimente.

[1] Sonderausgabe „Biomoleküle in der Gasphase“ *Eur. Phys. J. D* **20**(3), 309–626 (2002)

[2] Sonderausgabe „Bioaktive Moleküle in der Gasphase“ *Phys. Chem. Chem. Phys.* **6**(10), 2543–2890 (2004)

[3] H.L. Bethlem und G. Meijer, *Int. Rev. Phys. Chem.* **22**, 73–128 (2003)

MO 22.4 Sa 10:30 Poster HU

TOWARDS MAGNETIC TRAPPING OF ULTRACOLD POLAR MOLECULES — •Michael Stoll[1,2], Joost M. Bakker[1,2], Gerard Meijer[1] und Achim Peters[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Germany

Buffer gas loading and subsequent magnetic trapping of neutral molecules is a powerful tool for the creation of dense samples of ultracold molecules and is applicable to a wide variety of paramagnetic species. Such dense samples of ultracold molecules can form a starting point for experiments aimed at studying the formation of a molecular quantum gas, to perform ultra-high resolution spectroscopic measurements, and to test fundamental physics or interactions between ultracold molecules.

In this project we aim to create dense samples of neutral paramagnetic molecules by means of buffer-gas loading and trapping inside a superconducting quadrupole magnet using a ^{3}He-^{4}He dilution refrigerator. We report on the progress and test of the experiment using atomic Chromium. We also discuss the perspectives for cooling and trapping OH and NH radicals and present results from related precursor experiments.

MO 22.5 Sa 10:30 Poster HU

Down-scaling of molecule-optical elements by means of microstructure arrays — •Stephan Schulz, Hendrick Bethlem, Horst Conrad, and Gerard Meijer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

As previously shown, dipolar molecules can be manipulated by inhomogeneous electric fields making use of the Stark interaction. It has been demonstrated that fast switching of fields in the order of 100 kV/cm allows deceleration, focusing, and trapping of a variety of molecules with a static dipole moment. The electrode structures used have spatial extensions in the range mm to cm. As the applicable forces depend only on the electric field strength, a down-scaling to μm distances provide a reduction of the necessary voltages from $\sim$10 kV to some 100 V. Moreover, as μm scale electrode arrays on substrates are easily achievable within the state-of-the-art techniques, it is very attractive to do molecule-optics with a chip size device. We have recently demonstrated [1] that slow ND_3 molecules are reflected from a 2x2 mm^2 planar array of line electrodes separated by 20 μm loaded with alternating voltages ($\sim$300 V), such acting as an electrostatic mirror for polar molecules. In extending the down-scaling approach to more complicated structures, we will present a model calculation of the field geometry and molecule trajectories for an on-chip decelerator discussing possible spatial configurations.

[1] Stephan Schulz et al., 2004, *Phys. Rev. Lett.* **93**, 020406.

MO 22.6 Sa 10:30 Poster HU

EXPERIMENTAL STUDY OF COLD ATOM-MOLECULE COLLISIONS IN A MAGNETIC TRAP — •Sophie Schlunk[1], Allard Mosk[2], Wieland Schöllkopf[1] und Gerard Meijer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]University of Twente, Enschede, The Netherlands

Cooling and trapping of molecules is difficult mainly because laser cooling, in contrast to atoms, has not been applicable to molecules. In addition, cooling a molecular gas by forced evaporation or by sympathetic cooling with atoms has not yet been demonstrated at sub-millikelvin temperatures. Its efficacy depends on the rates of elastic and inelastic (trap-loss) collisions. For molecule-molecule as well as for most atom-molecule collisions the corresponding low temperature cross sections cannot be predicted by theory because of uncertainties in the best-known interaction potentials. We plan to experimentally study cold atom-molecule collisions. A large elastic-to-inelastic collision-rate ratio is prerequisite to sympathetically cool molecules with atoms in a 2-species trap.

We have cooled Rb-atoms in a standard magneto-optical trap (MOT) loaded from a Zeeman-slower. After transfer to and adiabatic compression in a magnetic trap a density on the order of 10^{11} atoms/cm^3 and a temperature of about 1 mK is expected. We plan first to study collisions between Rb-atoms and molecules at well defined and variable relative velocities by colliding a thermal or Stark-decelerated beam of heteronuclear molecules (e.g. NO, CO*, or ND_3) with the cold Rb-atom target. Eventually, we plan to explore sympathetic cooling of heteronuclear polar molecules with Rb-atoms confined simultaneously in 2-species trap.

MO 22.7 Sa 10:30 Poster HU

Fragmentation dynamics of polycyclic aromatic hydrocarbons — •Adalbert Ding, Christian Lenski, and Michael Lenski — Technische Universität Berlin, Optisches Institut, Sekr. P1-1, Strasse des 17. Juni 135, D-10623 Berlin

Most favoured theories concerning diffuse interstellar bands propose that the observed radiation originates from infrared fluorescences of vibronic highly excited polycyclic aromatic hydrocarbons (PAHs).

Photodissociation of PAHs has been shown to be the principal process competing with radiative relaxation of these PAHs. Due to their high resilience towards decomposition PAHs are attractive compounds for photoionization studies.

Light from the Berlin synchrotron BESSY was used to investigate the fragmentation of various PAHs by means of standard ionisation and coincidence techniques. By evaporation of the solid substances in an oven an effusive beam of target molecules was produced. After having been ionized using photon energies between 10 eV and 30 eV the fragmentation of these PAHs has been analyzed by means of time of flight mass spectrometry.

At sufficiently high photon energies dissociation via splitting off H-atoms and C_xH_y-fragments is observed. The critical energies are determined and compared with appropriate values from electron bombardement ionisation. Experimentally taken breakdown curves are compared with RRKM calculations.

MO 22.8 Sa 10:30 Poster HU

DFT-Investigations of coalescence behaviour of Si_4 and Si_7 clusters on surfaces — •Wolfram Quester[1], Dominik Fischer[2,1], and Peter Nielaba[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]IBM Zürich Research Laboratory, Säumerstraße 4, 8803 Rüschlikon

Experimental results show that Si_4 and Si_7 clusters do not form islands of bulk Si on weakly interacting surfaces (HOPG). We investigated the coalescence behaviour using Density Functional Theory implemented in the CPMD code (www.cpmd.org). Potential energy curves of two approaching Si_4 clusters on two reaction channels were calculated. It could be shown that there exists a fusion barrier which is higher than room temperature. These calculations will be extended to Si_7 clusters.

To get information about the influence of the substrate a calculation of a Si_4 cluster on a gold surface was perfomed. This simulation revealed that gold is not suited as substrate for depositing Si clusters.

MO 22.9 Sa 10:30 Poster HU

Reaction of mass selected vanadium oxide cluster ions with oxygen, sulfur dioxide and water. — •Mathias Brümmer[1], Sara Fontanella[1], Cristina Kaposta[1], Gabriele Santambrogio[1], Ludger Wöste[1], and Knut Asmis[2] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Fritz Haber Institut der Max Planck Gesellschaft, Abteilung Molekülphysik, Faradayweg 4-6, 14195 Berlin

Using a temperature-controllable frequency ion trap, we investigated the reaction kintetics of vanadium oxide cluster anions and cations with oxygen, sulfur dioxide and water under multi-collision conditions. The ion trap is inserted into a tandem quadrupole mass spectrometer to investigate mass selected cluster ions. By mass selected detection of the formed reaction products as a function of trap temperature and trapping time we were able to get informations about reaction paths and the kinetics of product formation.

MO 22.10 Sa 10:30 Poster HU

Influence of size and composition on the reaction kinetics of binary gold-silver cluster anions in an rf-ion trap — •Denisia Popolan, Jan Hagen, Liana D. Socaciu, Mihai E. Vaida, Bruno S. Schmidt, Thorsten M. Bernhardt, and Ludger Wöste — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

Small metal clusters were subject of many experimental and theoretical investigations in the last decade because of their fascinating size-dependent physical and chemical properties, which differ significantly from those of the atom and the bulk. The investigation of small charged clusters in the gas phase may even add to an understanding of catalytic reaction mechanisms. In contrast to the extensively studied electronic and structural properties of pure gold and silver clusters in the gas phase and on surface, considerably less information is available about the bimetallic silver-gold clusters, although supported bimetallic particles are promising candidates for industrial heterogeneous catalysis. In this context, we have investigated the reactive behaviour of binary $Ag_nAu_m^-$ clusters in an rf-ion trap setup. It was found that $AuAg^-$ reacts with O_2 reactive gas, and remains inert against CO. Surprisingly, the mixed silver-gold trimers present non-reactive character toward both, O_2 and CO. A comparison between reaction behaviour of pure Ag_n^-, Au_m^- and mixed $Ag_nAu_m^-$ in the presence of O_2 and CO reactive gas will be presented.

MO 22.11 Sa 10:30 Poster HU

Photoelectron spectroscopy of Na_n^- with n=3-1600 — •Oleg Kostko and Bernd v.Issendorff — Fakultät für Physik, Universität Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg

Size-selected sodium cluster anions with temperatures of T=100 K have been studied by photoelectron spectroscopy in a very broad size range. The spectra exhibit clear structures which in combination with ab initio DFT calculations can be used to identify the geometry of the clusters. Icosahedral symmetry prevails, but other motifs are observed as well. A simple new evaluation technique is introduced which measures the modulation of the photoelectron spectra. Hereby one can compress the whole data set into one single graph, which allows one to easily identify electronic and geometric shell closings.

MO 22.12 Sa 10:30 Poster HU

Angular resolved cluster photoelectron spectroscopy — •Christof Bartels, Christian Hock, and Bernd v.Issendorff — Fakultät für Physik, Universität Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg

Measuring the angular distribution of photoelectrons after photoionization or detachment yields information about the nature of the electron orbitals as well as the excitation process. A new imaging spectrometer has been constructed which can be used for high resolution angular resolved photoelectron spectroscopy on size-selected cluster anions and cations. It will be employed for a number of different studies. Firstly it is planned to do nanosecond spectroscopy on metal and semiconductor clusters, in order to study details of the electronic structure of this particles. Secondly it will be used for femtosecond spectroscopy of metal clusters, in order to clarify details of multiphoton electron detachment as well as to measure ultrafast relaxation times. First results are presented.

MO 22.13 Sa 10:30 Poster HU

Femtosecond photoelectron spectroscopy of sodium clusters — •Abdollah Malakzadeh, Christian Hock, Christof Bartels, Raphael Kuhnen, and Bernd v.Issendorff — Fakultät für Physik, Universität Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg

Recently we have shown that the electron gas in a free sodium cluster can be heated by a single fs-laser pulse to temperatures high enough for thermal electron emission to occur. This emission can be described by a simple model: the laser excites the collective motion of the electrons (the plasmon), which after a very short time (a few fs) decays into single electron-hole excitations. Due to the strong electron-electron interaction within a short time this nonthermal energy distribution of the electrons is transformed into a thermal one. The electron gas then cools by electron-phonon coupling. Time-resolved pump-probe photoelectron and photofragmentation spectroscopy has been applied to measure the electron-phonon-coupling constant as a function of cluster size. This has been done using relatively long laser pulses ($\tau \approx 200$ fs). In order to obtain more information about the early stages of the excitation, shorter laser pulses are necessary. Therefore a NOPA (noncollinear optical parametric amplifier) has been constructed, which allows the production of wavelength tunable, short ($\tau < 50$ fs) laser pulses, as well as a hollow capillary compressor. The performance of these devices and first results for sodium clusters are discussed.

MO 22.14 Sa 10:30 Poster HU

Infrared Photodissociation Spectroscopy of Gas-Phase Mass-Selected Vanadium Oxide Cluster Anions — •Gabriele Santambrogio[1], Mathias Brümmer[1], Joachim Sauer[2], Ludger Wöste[1] und Knut Asmis[3] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195, Berlin — [2]Institut für Chemie, Humboldt-Universität Berlin, Unter den Linden 6, 10099, Berlin — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Molekülphysik, Faradayweg 4-6, 14195, Berlin

Infrared photodissociation spectroscopy is one of the few methods available to investigate the structure of selected clusters in the gas-phase. Here we present the first infrared spectra of gas-phase mass-selected vanadium oxide cluster anions in the spectral region from 6 to 16 microns. Anions were produced by laser vaporization and excited using tunable infrared radiation from a free electron laser (FELIX, at the FOM Institute for Plasma Physics in Nieuwegein, NL). We investigated clusters from $V_2O_6^-$ up to $V_8O_{20}^-$. By comparison with DFT calculations we were able to unambiguously determine the structure of the clusters. The structures of the small anions are similar, though not identical, to those already observed for the cationic species, consisting of a planar central V-O-V-O ring. For larger anions we observed for the first time the predicted highly symmetric cage structures. Furthermore, we found a size-dependent charge localization in polyhedral cage structures of $(V_2O_5)_n$ clusters (n=2,3,4).

MO 22.15 Sa 10:30 Poster HU

Melting of Cluster: where do the Magic Numbers come from? — •Christian Hock[1], Hellmut Haberland[1], Thomas Hippler[1], Jörn Donges[1], Oleg Kostko[1], Martin Schmidt[2], and Bernd v.Issendorff[1] — [1]Department of Physics, University of Freiburg, 79104 Freiburg, Germany — [2]Laboratoire Aimé Cotton, CNRS II, 97406 Orsay, France

Melting temperatures of Na clusters show size dependent fluctuations which have resisted interpretation so far. We discuss that these temperatures in fact cannot be expected to exhibit an easily understandable behaviour. The energy and entropy differences between the liquid and solid clusters turn out to be much more relevant paramters. They exhibit pronounced maxima which correlate well with *geometrical* shell closings, demonstrating the importance of geometric structure for the melting process. Icosahedral symmetry dominates, a conclusion corroborated by new photoelectron spectra measured on cold cluster anions. In the vicinity of the geometrical shell closings the measured entropy is in good agreement with a simple combinatoric model.

MO 22.16 Sa 10:30 Poster HU

Doppelionisationsmechanismen kleiner Cluster — •T. Jahnke[1], A. Czasch[1], M. Schöffler[1], S. Schössler[1], A. Knapp[1], M. Käsz[1], J. Titze[1], C. Wimmer[1], K. Kreidi[1], R. E. Grisenti[1], A. Staudte[1], O. Jagutzki[1], U. Hergenhahn[2], H. Schmidt-Böcking[1] und R. Dörner[1] — [1]Institut für Kernphysik, J. W. Goethe-Universität Frankfurt am Main, August-Euler-Str. 6, D-60486 Frankfurt, Germany — [2]Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, D-85748 Garching, Germany

In der letzten Zeit konnte Ïnteratomic Coulombic Decay”(ICD) an Clustern eindeutig experimentell nachgewiesen werden. In der vorliegenden Arbeit, wird an einem Neon Dimer gezeigt, daß auch andere Doppelionisationsmechanismen in Clustern auftreten können.

Die vorgestellten Ergebnisse wurden mit Hilfe von multikoinzidenter Impulsspektroskopie (COLTRIMS) am BESSY II gemessen: Alle 4 Fragmente eines doppelionisierten Dimers (2 Neonionen und 2 Elektronen) wurden für jedes Photoionisationsereignis nachgewiesen. Die hieraus erhaltenen hochdifferenziellen Wirkungsquerschnitte können einzelnen Ionisationsmechanismen zugeordnet werden und werden hier vorgestellt.

MO 22.17 Sa 10:30 Poster HU

Absorption von Mg-Atomen in Heliumtropfen — •Andreas Przystawik, Sebastian Göde, Josef Tiggesbäumker und Karl-Heinz Meiwes-Broer — Institut für Physik, Universitätsplatz 3, 18051 Rostock

Bei einer Düsenstrahlexpansion von Helium ins Vakuum entstehen ultrakalte Heliumtröpfchen, die beim Passieren einer Pickup-Zelle Atome aus einem Dampf niedriger Dichte aufnehmen können [1].

Laserinduzierte Fluoreszenzspektroskopie sowie resonante Zwei-Photonen-Spketroskopie an Magnesiumatomen zeigen, dass sich Magnesiumatome im Inneren des Tropfens befinden [2,3]. Die Aufspaltung des Überganges in zwei Komponenten wird im Rahmen eines modifizierten Blasenmodells als Quadrupolschwingung des umgebenden Heliums aufgrund der nichtsphärischen Elektronenverteilung des angeregten Atoms gedeutet. Neue Messungen zeigen jedoch, daß die relative Intensität der beiden Komponenten durch die Wahl der Bedingungen, insbesondere durch den Dampfdruck in der Pickup-Zelle, beeinflußt werden kann.

[1] A. Bartelt, J.D. Close, F. Federmann, N. Quaas und J.P. Toennies, Phys. Rev. Lett. **77**, 3525 (1996)
[2] J. Reho, U. Merker, M.R. Radcliff, K.K. Lehmann und G. Scoles, J. Chem. Phys. **112**, 8409 (2000)
[3] T. Diederich, J. Tiggesbäumker, K.-H. Meiwes-Broer, J. Chem. Phys. **116**, 3263 (2001)

MO 22.18 Sa 10:30 Poster HU

Photoioniation von Alkaliclustern auf Helium-Nanotröpfchen — •O. Bünermann, S. Cunovic und F. Stienkemeier — Fakultät für Physik,Universität Bielefeld,Universitätsstr. 25, 33615 Bielefeld

Auf der Oberfläche von Helium-Nanotröpfchen ist es möglich, Moleküle und kleine Cluster aus Alkaliatomen zu bilden. Wir haben diese mittels resonanter 2-Photonen Photoionisation untersucht, um Aussagen über elektronische Anregungen der Cluster zu erhalten. Die Photoionisation besitzt dabei gegenüber Fluoreszenzmethoden den Vorteil, dass sie auch Zustände detektiert, die strahlungslos zerfallen. Zudem können die erzeugten Ionen massenselektiv nachgewiesen werden und somit zusätzlich Aussagen über die Fragmentation der Alkalicluster nach einer Anregung gemacht werden. Im Fall von Natrium und Kalium-Dimeren wurden so bisher experimentell nicht zugängliche Triplettübergänge vermessen und erste Absorptionen kleinerer Cluster in der Heliumumgebung charakterisiert.

MO 22.19 Sa 10:30 Poster HU

Depletion-Spektroskopie von dotierten Heliumnanodroplets mit einem cw-optoparametrischen Oszillator im Bereich von 3008-3039 cm^{-1} — •Stephan Rudolph, Götz Wollny, Markus Ortlieb, Klaus von Haeften und Martina Havenith — Ruhruniversität Bochum

Bei einer Düsenstrahlexpansion werden Heliumnanodroplets erzeugt, in denen Moleküle bei 0,37 K eingelagert und spektroskopisch untersucht werden können.

Als neue Strahlungsquelle für das mittlere Infrarot wird ein cw-optoparametrischen Oszillator (OPO) vorgestellt, der die Spektroskopie von ultrakalten Gasen im mittleren Infrarot-Bereich des elektromagnetischen Spektrums ermöglicht. Der OPO stellt eine cw-Strahlungsquelle mit hoher Leistung (max. 2,9 W), hoher Durchstimmbarkeit (2,9-3,9 μm) und schmaler Linienbreite ($\leq$ 1 MHz) dar. Es konnten auf Grund dieser hohen Leistung erstmalig Sättigungseffekte der Anregung bei der Spektroskopie von Methan in Heliumnanodroplets im Bereich von 3008-3039 cm^{-1} gezeigt werden.

MO 22.20 Sa 10:30 Poster HU

Full relativistic density-functional calculations of 114X and PbX dimers (with X=O, Pd, Pt, Au) — •Cristina Sarpe-Tudoran[1], Josef Anton[1], Wolf-Dieter Sepp[1], Burkhard Fricke[1], and Valeria Pershina[2] — [1]Institut für Physik, Universität Kassel, D-34109 Kassel, Germany — [2]Gesellschaft für Schwerionenforschung, D-64291 Darmstadt, Germany

A detailed study of the electronic structure and bonding of the 114X and PbX molecules (with X=Au,Pd,Pt,O) was carried out using a fully relativistic 4-component density-functional method. The intention of this study is to learn more about the differences between the homologues of the 6th and 7th row elements [1,2].

For the dimers considered in the work, the potential energy curves, the vibrational frequencies, the corresponding binding energies and bond lengths are presented. To determine the character of the binding the Mulliken population, the total and partial Density of States as well as the total and partial Overlap Population are analyzed.

[1] W. Liu and C. van Wüllen, J. Chem. Phys. 110 3730 (1999) [2] J. Anton, B. Fricke, P. Schwerdfeger, Chem. Phys. in press

MO 22.21 Sa 10:30 Poster HU

Käfigeffekt und Dissoziation im System $Br_2 : Ar$ — •Heide Ibrahim, Markus Gühr und Nikolaus Schwentner — Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

Wir untersuchen Br_2-Moleküle in kristallinem Argon mittels fs-Pump-

Probe Spektroskopie. Dazu verwenden wir durchstimmbare Laserpulse (470 bis 650 nm) mit einer Pulslänge von teilweise unter 50 fs. Für den Nachweis der laserinduzierten Fluoreszenz werden verschiedene Ladungstransfer-Emissionen im UV-Bereich vorgestellt.

Aus der Dynamik der Schwingungswellenpakete im B-Zustand ($^3\Pi_0$) leiten wir mit Hilfe eines RKR-Formalismus die intramolekularen Molekülpotentiale bis über die Gasphasen-Dissoziationsgrenze hinaus ab und diskutieren daraus den Einfluß des Argonkäfigs. Die Wellenpaketdynamik liefert bei Variation der Pump- und Probeenergie auch die Schwingungsenergierelaxation. Sie wurde insbesondere im Bereich der Kreuzung mit repulsiven Zuständen in Hinblick auf eine matrixinduzierte Verstä rkung der Prädissoziation untersucht.

Eine permanente Dissoziation wird über die Kinetik des Ausbleichens charakterisiert. Die Intensitätsabhängigkeit kennzeichnet die relevanten Übergänge; Reorientierung bei der Rekombination wird mit Hilfe von Polarisationsstudien diskutiert.

MO 22.22 Sa 10:30 Poster HU

Coherence of molecules in condensed phase: Cl_2 in Ar — •Mizuho Fushitani, Matias Bargheer, Markus Gühr, and Nikolaus Schwentner — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee, 14195 Berlin, Germany

Vibrational and electronic coherence of Cl_2 molecules in solid Ar was studied by using a fs pump probe technique. We observed wavepacket oscillations with two different periods: 300fs and 500fs. The shorter round trip time is assigned to the vibrational motion of the B state of Cl_2 while the longer period is due to the zone boundary lattice vibration of solid Ar. The same 500fs oscillation was also observed in the system of Br_2/Ar[1], which indicates that the modulation should be attributed to the host dynamics, not to the chromophore.

The electronic coherence between the electronic ground state and the excited B state of Cl_2 in solid Ar was studied by using a phase locked pulse pair (PLPP) as a pump pulse. Depending on the relative phase of the PLPP after each vibrational period, more or less population can be transferred to the B state if molecules keep the phase information. The population created by a PLPP was transferred to an ion-pair manifold state of Cl_2 by a probe pulse, and the LIF from the state was monitored as a function of the delay between the PLPP. We observed vibrational recurrence around 210 fs in the LIF interferogram using a PLPP at 535 nm. The contribution of zero phonon line and phonon side band to the recurrence will be discussed.

[1] M. Gühr and N. Schwentner, PCCP submitted.

MO 22.23 Sa 10:30 Poster HU

Aufbau und Betrieb einer Apparatur zur Untersuchung der Photodissoziation von Alkali-Hologeniden im Molekülstrahl — •Falk Königsmann[1], Marcel Dickow[1], Waldemar Unrau[1], Tobias Liebig[1], Dieter Zimmermann[1], Konstantin Korovin[2] und Oleg Vasyutinskii[2] — [1]Institut für Atomare Physik und Fachdidaktik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg

Die Analyse der Spin-Polarisation atomarer Photofragmente in Abhängigkeit vom Rückstoß-Winkel nach der Photodissoziation stellt eine produktive Methode zur Untersuchung des Photodissoziationsprozesses dar. Vorgestellt wird eine Apparatur, die es möglich macht, diesen Prozess bei unterschiedlichen Wellenlängen und Polarisierungen des ultravioletten Dissoziationslichtes zu untersuchen. Es soll durch geeignete Wahl der Wellenlänge des dissoziierenden Lichts versucht werden, nur molekulare Zustände anzuregen, die in die Grundzustände von Na und I zerfallen.

Dazu wird NaI bei einem Restdruck von 10^6 mbar in einem widerstandsbeheiztem Ofen verdampft und mit einem Excimer-Laser-gepumpten Farbstoff-Laser mit Frequenz-Verdoppelungseinheit dissoziiert. Die Absorption und Dispersion des entstehenden atomarem Natriums wird durch Scannen eines single-mode Ring-Dye-Laser um die Natrium D-Linie untersucht.

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3D-Imaging der Photodissoziation von Schwefeldichlorid — •Oliver Ott[1], Christof Maul[1], Alexei Chichinin[1,2] und Karl-Heinz Gericke[1] — [1]Institut für Physikalische und Theoretische Chemie, TU Braunschweig, Hans-Sommer-Str. 10, 38106 Braunschweig — [2]Institute of Chemical Kinetics and Combustion, 630090 Novosibirsk, Russland

Die Photodissoziation von Schwefeldichlorid wurde mittels der in Braunschweig entwickelten dreidimensionalen Imaging-Methode untersucht, die die zustandsaufgelöste Beobachtung des dreidimensionalen Teilchenimpulses individueller Fragmente erlaubt. Chloratome im $^2P_{3/2}$-Grundzustand sowie im angeregten ($^2P_{1/2}$) Spin-Bahn-Zustand wurden mittels resonant erhöhter Multiphotonenionisation (REMPI) und eines orts- und zeitauflösenden delay-line-Detektors nachgewiesen. Geschwindigkeitsverteilungen und das räumliche Anisotropieverhalten belegen, dass die Dissoziation direkt über einen $^1B_1$-Zustand des Muttermoleküls erfolgt. Die experimentellen Beobachtungen bestätigen theoretische Berechnungen angeregter elektronischer Zustände des Muttermoleküls. Bestehende Diskrepanzen hinsichtlich des Absorptionsspektrums von SCl_2 konnten geklärt werden.

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Photoexcitation and Photofragmentation of the 3d- transition metal compounds $FeCl_2$ and $FeBr_2$ — •Mohamed Al-Hada[1], Michael Martins[2], Tobias Richter[1], Peter Zimmermann[1], Ömer Görgülüer[3], Ali Tutay[3], and Mehtap Yalcinkaya[3] — [1]Institut für Atomare Physik und Fachdidaktik, Technische Universität Berlin,Hardenbergstraße 36, 10623 Berlin, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 2276 Hamburg, Germany — [3]Science Faculty, Istanbul University, 34459 Istanbul, Turkey

The atomic absorption spectrum of the 3d element Fe in the region of the 3p excitation is dominated by strong resonances (giant resonances) due to discrete transitions $3p^6\ 3d^6$ to $3p^5\ 3d^7$ [1]. This is caused by the large overlap of the 3p and 3d wave functions. The atomic Fe 3p photoelectron spectrum in a similar way is determined by the 3p-3d interaction resulting in a large splitting of the $3p^{-1}$ multiplet [2]. It is a challenging task to probe this interaction of an inner shell 3p hole with the 3d valence electrons for the Fe compounds $FeCl_2$ and $FeBr_2$ due to fragmentation processes which act as complex dominant processes in these molecules.

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Photo-induced structural changes in organic single crystals — •Jav Davaasambuu, Gerhard Busse, and Simone Techert — Max-Planck-Institute for biophysical Chemistry, Am Fassberg 11, 37077 Goettingen

Photo-induced structural changes in organic single crystals of 2-benzyl-5-benzylidenecyclopentanone[1] and 2,4-dichloro trans-cinnamic acid[2] have been investigated using high resolution x-ray diffraction. Single crystal to single crystal photodimerisations of these crystals are performed by irradiation monomer crystals with a high-pressure mercury lamp. The crystal structures of the monomer and the dimer for these crystals were solved by direct methods using the SHELXTL program package. In these single crystals a cyclobutane ring formed from parallel two C=C double bonds of neighbouring molecules by light irradiation. It was found that the variations of the unit cell parameters of these crystals are very small(much less than 2%). In this contribution we present our preliminary results for the photoinduced dimerisation in the single crystals.

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MO 22.27 Sa 10:30 Poster HU

Photoionization and photodissociation of HCl near 236 nm using three-dimensional ion imaging — •Niels Gödecke[1], Alexey Chichinin[2], Christof Maul[1], and Karl-Heinz Gericke[1] — [1]Institut für Theoretische und Physikalische Chemie, TU Braunschweig, D-38106 Braunschweig — [2]Institute of Chemical Kinetics and Combustion, 630090 Novosibirsk, Russia

The electronically excited state HCl ($B^1\Sigma^+, J' = 0$), denoted HCl^*, has been prepared by two-photon resonant absorption of ground state HCl at 236.000 nm and at 238.719 nm, respectively. The consequent one- or two-photon excitation at the same wavelength results in production of H^+, Cl^+ and HCl^+ ions. The speed distributions and anisotropy parameters β for these ions have been determined by three-dimensional photofragment ion imaging technique. It has been shown that the ions are produced via different pathways, which may be denoted as resonance enhanced multi-photon ionization (REMPI) $2 + 1_i, 2 + 1 + 1_i, 2 + 1_i + 1$, and $2 + 2$, where the index i labels the ionizing photon. The measured velocity distribution for HCl^+ characterises the electron recoil in the photoionization of HCl^+ in other cases the information on the photodissociation steps was obtained.

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Detailed analysis of normal and resonant Auger spectra in H_2S — •M Poiguine[1], R Püttner[1], M Martins[2], V Pennanen[2], M Jurvansuu[2], Y Jiang[1], S Aksela[2], and G Kaindl[1] — [1]Freie Universität Berlin, D-14195 Berlin — [2]University of Oulu, Department of Physical Sciences, 90401 Oulu, Finland

High-resolution S $2p^{-1}$ photoelectron spectra (PES) and $2p^{-1} \rightarrow X^1A_1(2b_1^{-2})$ normal Auger electron spectra (AES) of H_2S have been measured using different photon energies. These spectra were fitted simultaneously with a model that includes spin-orbit and ligand-field splittings, post-collision interaction, and vibrational fine structures in the core-excited and final states, as well as vibrational and electronic lifetime interference. This elaborated fit analysis resulted in an excellent agreement with the spectra and allowed to derive detailed information about the geometry and potential energy surfaces in the core-hole and final states. In addition, detailed analysis of photoabsorption spectra in the energy region between 167.3 and 168.3 eV are also presented, along with the corresponding resonant Auger spectra.

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Mit dem TTM2-F Potential zum kleinsten Eiskristall — •Bernhard Bandow und Bernd Hartke — Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, 24118 Kiel

Die Anzahl der lokalen Minima der Energiehyperfläche des Konfigurationsraumes von Clustern wächst exponentiell mit der Clustergröße. Gerade bei rechenintensiven Potentialen ist daher die mit vertretbarem Zeitaufwand untersuchbare Clustergröße gering. Unsere Untersuchungen von Wasserclustern mit n¡=150 geschehen mit Hilfe einer eigenen massiv parallelen, auf MPI (Message Passing Interface) aufsetzenden Implementierung eines Evolutionären Algorithmus (EA) zur globalen Geometrieoptimierung.

Zum Einsatz kommt dabei das TTM2-F Potential. Es läßt Verzerrungen der als polarisierbar angenommenen Wassermoleküle vermöge variabler OH-Bindungslänge und variablem HOH-Bindungswinkel zu. Ferner sind die Partialladungen nicht punktförmig, sondern verschmiert und Vielteilchenterme werden iterativ berücksichtigt. Daher ist der Rechenaufwand erheblich größer als es für die von starren Molekülen ausgehenden Potentiale der Fall ist. Von diesen ist das TIP4P-Potential der prominenteste Vertreter und die Referenz für unsere Untersuchungen.

Basierend auf den bisherigen Resultaten zeigen sich für kleine Cluster (n¡=17) Minimalstrukturen, die nur aus Oberflächenmolekülen bestehen. Bis zu einer Größe von n=21 findet ein Übergang zu Clathratstrukturen statt, die in ihrem Innern ein einzelnes Molekül beherbergen. Darüber findet man mit wachsendem n stufenweise mehr interne Moleküle. Ein erster Vergleich mit Ausschnitten aus Eis der Modifikationen Ic, Ih, VII, VIII, IX zeigt wenigstens bis n=100 einen energetischen Vorteil zugunsten der optimierten Clusterstrukturen.

Die bisher einzige andere systematische Untersuchung spricht für eine Gitterstruktur im Inneren der Cluster ab etwa n=120, stützt sich dabei jedoch auf das TIP4P-Potential. Somit bleibt die Frage zu klären, ob und ab welcher Größe auch im Inneren der auf dem TTM2-F-Potential basierenden Cluster eine Eisstruktur anzutreffen ist.

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High-resolution resonant Auger (RA) spectra of high-n $3d^{-1}nl\lambda$ excitations in HBr — •R. Püttner[1], Y. F. Hu[2], G. M. Bancroft[3], A. Kivimäki[4], M. Jurvansuu[4], H. Aksela[4], and S. Aksela[4] — [1]Freie Universität Berlin, D-14195 Berlin — [2]Canadian Light Source Inc., University of Sasketchewan, Saskatoon, SK, Canada — [3]University of Western Ontario, London, On, Canada — [4]University of Oulu, 90401 Oulu, Finland

High-resolution RA spectra of transitions to the non-dissociative final states $4p\pi^{-2}nl\lambda$ of HBr subsequent to $3d^{-1}ml\lambda$ excitations are presented. The spectra subsequent to the $3d^{-1}5s, 5p$ excitations can be described by the splitting of the $4p\pi^{-2}$ final state and a coupling of the Rydberg electron, with little vibrational fine structure. However, the spectra due to $3d^{-1}7p, 8p$ excitations exhibit complexe features which can be explained with RA transitions to a number of different final states in combination with a vibrational profile for each transition similar to that of the $3d^{-1} \rightarrow 4p\pi^{-2}$ normal Auger process. The observed number of final states cannot be explained with the spectator/shake model for RA spectra but requires the consideration of non-monopole transitions.