

## MO 17: Elektronische Spektroskopie

Zeit: Dienstag 14:00–19:00

Raum: Poster C1

MO 17.1 Di 14:00 Poster C1

**High resolution Fourier transform spectroscopy on LiRb** — ●ALEXANDER STEIN<sup>1</sup>, ASEN PASHOV<sup>2</sup>, MILENA IVANOVA<sup>2</sup>, HORST KNÖCKEL<sup>1</sup>, and EBERHARD TIEMANN<sup>1</sup> — <sup>1</sup>Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover — <sup>2</sup>Department of Physics, Sofia University, 5 J. Bourchier blvd., 1164 Sofia, Bulgaria

The LiRb molecule is one of the few heteronuclear alkali metal molecules (along with those containing one Fr atom), for which accurate spectroscopic information is still missing. On the other hand it is one of the most polar among the alkali molecules and is surely of interest in experiments with mixtures of cold atoms (e.g. D. DeMille, Phys. Rev. Lett. 88, 067901 (2002)). We report the first high resolution observation of laser-induced fluorescence in the LiRb molecule. Abundant experimental information is collected with a typical resolution of 0.03 cm<sup>-1</sup> applying a Fourier-transform spectrometer. The present status of the analysis and preliminary potentials for the X<sup>1</sup>Σ<sup>+</sup> ground state and the two lowest <sup>1</sup>Π states are presented.

MO 17.2 Di 14:00 Poster C1

**High resolution Fourier transform spectroscopy on Sr<sub>2</sub>** — ●ALEXANDER STEIN, HORST KNÖCKEL, and EBERHARD TIEMANN — Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover

Strontium actually is a candidate for a new and more precise frequency standard (e.g. I. Courtillot et al., Phys. Ref. A 68, 030501(R) (2003)). Hence there is a high interest in cooling and trapping of cold strontium atoms (M. Yasuda and H. Katori, Phys. Rev. Lett. 92, 153004 (2004)). At the moment there are no sufficiently precise potentials available for the Sr<sub>2</sub> molecule allowing the calculation of collisional properties as the scattering length.

We report on new spectroscopic investigations using a heat pipe setup. The current status of the experiment and improved potentials of the X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> ground state and the excited 2(A)<sup>1</sup>Σ<sub>u</sub><sup>+</sup> state will be presented.

MO 17.3 Di 14:00 Poster C1

**Transient Spectroscopy of UV excited flavone and substituted porphyrins: Triplet-Triplet absorption and comparison with theory** — ●GERNOT ENGLER<sup>1</sup>, DENNIS LÖWENICH<sup>1</sup>, KARL KLEINERMANN<sup>1</sup>, MARTIN KLEINSCHMIDT<sup>2</sup>, CHRISTEL MARIAN<sup>2</sup>, and SERGEJ KOVALENKO<sup>3</sup> — <sup>1</sup>Institute for Physical Chemistry, Heinrich-Heine-University, Universitätsstr. 1, D-40225 Düsseldorf, Germany — <sup>2</sup>Institute for Theoretical Chemistry, Heinrich-Heine-University, Universitätsstr. 1, D-40225 Düsseldorf, Germany — <sup>3</sup>Institute for Chemistry, Humboldt University of Berlin, Brook-Taylor-Strasse 2, D-12489, Berlin, Germany

We reinvestigated the triplet absorption of flavone in solvents with different polarity at excitation wavelengths of 266 nm and 355 nm. Strong solvent dependent shifts of the transient absorption spectrum can be explained by comparison with TDDFT/MRCI calculations. We also investigated the triplet absorption of tetraphenylporphyrin (TPP), tetracarboxyphenylporphyrin (TCPP) and tetrahydroxyphenylporphyrin (THPP) in cyclohexane and ethanol in the spectral range 280-800 nm and observed T1-TN absorption at 320, 370, 440 and 470 nm which could be assigned to specific transitions by comparison with TDDFT/MRCI calculations. TCPP and THPP showed transient absorption at similar wavelengths and similar T1- lifetimes of a few us. The rise times both of the flavone and porphyrin transients are < 20 ns pointing to very efficient S1-T1 intersystem crossing.

MO 17.4 Di 14:00 Poster C1

**Aufbau und Charakterisierung einer durchstimmbaren Kurzpuls Vakuu-UV Quelle für zeitaufgelöste Anregungs-Nachweis Experimente** — ●EGILL ANTONSSON, JÜRGEN PLENGE, ANDREAS WIRSING und ECKART RÜHL — Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Es wird eine Kurzpuls Vakuu-UV Strahlungsquelle vorgestellt, die auf der Emission eines laserinduzierten Plasmas beruht und kontinuierlich durchstimmbare Vakuu-UV Strahlung im Photonenenergiebereich 10-30 eV liefert. Der Aufbau des Anregungs-Nachweis Experiments beinhaltet ein Femtosekunden-Lasersystem (Pulsdauer: 85 fs; Pulsenergie: 30 mJ) zur Erzeugung des Plasmas auf der Ober-

fläche eines Wolfram-Drahtes, einen Vakuu- UV Monochromator zur Wellenlängenselektion und ein Flugzeit-Massenspektrometer. Es werden Anregungs-Nachweis Experimente vorgestellt, in denen der 1s<sup>2</sup>(<sup>1</sup>S) → 1s3p(<sup>1</sup>P) Übergang von Helium bei 23,09 eV angeregt wird. Der angeregte 1s3p(<sup>1</sup>P) Zustand wird nachfolgend mit Femtosekunden Laserpulsen (λ = 402, 5 nm) ionisiert. Aus dem zeitabhängigen Anstieg des He<sup>+</sup>-Signals wird die Pulsdauer der VUV-Strahlung ermittelt, wobei eine Pulsdauer von 75±20 ps erreicht wird. Mögliche Anwendungen der durchstimmbaren Kurzpuls Vakuu-UV-Quelle für zeitaufgelöste Anregungs-Nachweis Experimente werden diskutiert.

MO 17.5 Di 14:00 Poster C1

**CH-π interactions in Benzene-Acetylene clusters** — ●MATTHIAS BUSKER, THOMAS HÄBER, MICHAEL NISPEL, and KARL KLEINERMANN — Institut für Physikalische Chemie I, Heinrich Heine Universität Düsseldorf, Germany

CH-π interactions are interesting due to their importance for the stabilization of supramolecular aggregates, crystal packing, molecular recognition and folding of proteins. We present new gas phase results on medium-sized clusters of Benzene(B) with Acetylene(A) by using IR-UV double resonance spectroscopy for analysis. The investigated B<sub>1</sub>A<sub>1-4</sub> and B<sub>2</sub>A<sub>1-2</sub> aggregates were structurally assigned based on comparison of their infrared spectra with ab initio calculated frequencies and intensities and by taking the shift of their electronic spectra into account. The obtained cluster structures were compared with the basic structural units of BA 1:1 cocrystals obtained via x-ray analysis.

MO 17.6 Di 14:00 Poster C1

**Manifestation of lifetime vibrational interference in the decay of resonantly excited N\*O π\*(v) and NO\* π\*(v) states into the NO+ A state** — ●A. EHRESMANN<sup>1</sup>, W. KIELICH<sup>1</sup>, L. WERNER<sup>1</sup>, P.V. DEMEKHIN<sup>2</sup>, D.V. OMELIANENKO<sup>2</sup>, V.L. SUKHORUKOV<sup>2</sup>, K.-H. SCHARTNER<sup>3</sup>, and H. SCHMORANZER<sup>4</sup> — <sup>1</sup>Institute of Physics and CIN-SaT, University of Kassel, 34132 Kassel, Germany — <sup>2</sup>Rostov State University of Transport Communications, 344038 Rostov-on-Don, Russia — <sup>3</sup>I. Institute of Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany — <sup>4</sup>Department of Physics, Kaiserslautern University of Technology, 67653 Kaiserslautern, Germany

Dispersed fluorescence from the A-X(v') bands in the NO+ ion produced after de-excitation of the π\*(v) resonances of N\*O and NO\* has been measured in the spectral range of 118nm - 142 nm. This fluorescence results from the participator Auger decay of the π\* resonances into the NO+ A state. Ab-initio calculations of the transition probabilities between vibrational levels of the resonant state were used to explain the observed intensity dependences for the A(v')-X(v'') fluorescence bands on the exciting-photon energy across the inner-shell resonances and on both v' and v'' vibrational quantum numbers. The multiplet structure of the π\* resonance and lifetime vibrational interference explain the observed exciting-photon energy dependence of the observed A-X fluorescence bands.

MO 17.7 Di 14:00 Poster C1

**Isotope-specific and ultra-sensitive detection of nitric oxide: Application to exhaled air analysis** — CHRISTOPH MITSCHERLING, ●CHRISTOF MAUL, and KARL-HEINZ GERICKE — Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, 38106 Braunschweig, Hans-Sommer-Str. 10

Laser-induced fluorescence (LIF) and resonance-enhanced multiphoton ionization (REMPI) are extremely sensitive spectroscopic techniques for the investigation of low nitric oxide (NO) concentrations.

The mass selectivity of the REMPI method allows to identify spectral windows in which the most abundant isotopologues <sup>14</sup>N<sup>16</sup>O, <sup>15</sup>N<sup>16</sup>O, and <sup>14</sup>N<sup>18</sup>O can be monitored free from spectroscopic interference by each other. For this detection the A<sup>2</sup>Σ<sup>+</sup> ← X<sup>2</sup>Π<sub>g</sub> transition (NO γ bands) is used which is easily accessible in the ultraviolet wavelength range around 225nm.

Carefully selected rovibrational transitions are employed for the isotope-specific, ultra-sensitive detection of NO in exhaled air by laser induced fluorescence. Applications to on-line NO measurements for human breath analysis will be presented and discussed.

MO 17.8 Di 14:00 Poster C1

**Optical excitation and detection of nitrous oxide in the ultraviolet wavelength range** — ●CHRISTOF MAUL — Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, 38106 Braunschweig, Hans-Sommer-Str. 10

N<sub>2</sub>O is a widely used precursor molecule for O(<sup>1</sup>D) atoms, in particular for investigating the bimolecular reaction O(<sup>1</sup>D) + N<sub>2</sub>O → 2 NO which can be initiated with relative experimental ease by 193 nm laser radiation in a N<sub>2</sub>O sample. More often than not, such experiments are performed in supersonic expansions where low temperature and high number density favour the formation of N<sub>2</sub>O clusters which might affect the course of the reaction. Therefore, a method for characterization of the N<sub>2</sub>O sample under the conditions of a reactive scattering

experiment is desirable.

State selective excitation and detection of N<sub>2</sub>O through its Rydberg states is possible by resonance enhanced multi-photon ionization (REMPI) spectroscopy. Only two such studies have been published up to date, mainly relying on a (3+1)-REMPI scheme in the wavelength range from 350 nm to 370 nm. Data on (2+1)-REMPI excitation are less abundant and exist only for selected wavelength ranges and temperatures. Cluster formation has neither been investigated nor investigated.

The aim of the presented work is to characterize (2+1)-REMPI spectroscopy of N<sub>2</sub>O in the wavelength range from 235 nm to 245 nm under different experimental conditions, i.e. for room temperature and jet-cooled samples, and to explore the possibility of cluster detection.