

MO 5: Posters 1: Novelties in Molecular Physics

Time: Monday 17:00–19:00

Location: C/Foyer

MO 5.1 Mon 17:00 C/Foyer

Hartree-Fock calculation of the differential photoionization cross sections of small Li clusters — ●SERGEY A GALITSKIY¹, ANTON N ARTEMYEV¹, KARI JÄNKÄLÄ², BORIS M LAGUTIN³, and PHILIPP V DEMEKHIN¹ — ¹Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Department of Physics, University of Oulu, P.O. BOX 3000, 90014 Oulu, Finland — ³Research Institute of Physics, Southern Federal University, Stachki av. 194, 344090 Rostov-on-Don, Russia

Cross sections and angular distribution parameters for the single-photon ionization of all electron orbitals of Li_{2–8} are systematically computed in a broad interval of the photoelectron kinetic energies for the energetically most stable geometry of each cluster. Calculations of the partial photoelectron continuum waves in clusters are carried out by the Single Center method within the Hartree-Fock approximation. We study photoionization cross sections per one electron and analyze in some detail general trends in the photoionization of inner and outer shells with respect to the size and geometry of a cluster. The present differential cross sections computed for Li₂ are in a good agreement with the available theoretical data, whereas those computed for Li_{3–8} clusters can be considered as theoretical predictions.

MO 5.2 Mon 17:00 C/Foyer

Optical spectroscopy and structures of photo dissociated doped silicon clusters — ●BERTRAM K.A. JAEGER, JANINA LEBENDIG, NGUYEN X. TRUONG, ANDRE FIELICKE, and OTTO DOPFER — IOAP, TU Berlin, Germany

Doped Si clusters with their great variety in physical and chemical properties are promising candidates for optoelectronics, sensors or medicine. We study the photodissociation of C, N and O doped Si clusters and compare the spectra with quantum chemical calculations. A laser vaporization source produces ionic clusters, which are then irradiated with a tunable visible laser in the range from 410 to 580 nm. Photo-induced dissociation of the cluster changes the mass spectrum, which is recorded by a reflectron time-of-flight mass spectrometer. Calculated absorption spectra are compared to experimental data to access geometric or electronic parameters. With the help of genetic and basin-hopping algorithms the most stable and low-energy isomers are identified. Results are to be verified by existing studies of IR-UV two color ionization of neutral and doped Si clusters [1]. The basic principle of the experimental setup is shown with pristine and Ar-tagged Au₄₊ clusters. [1] N.X. Truong et al., Phys. Chem. Chem. Phys., 2014, 16, 40, 22364-22372

MO 5.3 Mon 17:00 C/Foyer

A molecular movie of Interatomic Coulombic Decay in NeKr — ●FLORIAN TRINTER¹, TSVETA MITEVA², MIRIAM WELLER¹, SEBASTIAN ALBRECHT¹, ALEXANDER HARTUNG¹, MARTIN RICHTER¹, JOSHUA WILLIAMS¹, AVERELL GATTON³, BISHWANATH GAIRE³, THORSTEN WEBER³, JAMES SARTOR⁴, ALLEN LANDERS⁴, BEN BERRY⁵, VASIL STUMPF², KIRILL GOKHBERG², TILL JAHNKE¹, and REINHARD DÖRNER¹ — ¹Institut für Kernphysik, Goethe-Universität, 60438 Frankfurt am Main, Germany — ²Theoretische Chemie, Physikalisches-Chemisches Institut, Universität Heidelberg, 69120 Heidelberg, Germany — ³Lawrence Berkeley National Laboratory, Chemical Sciences Division, Berkeley, California 94720, USA — ⁴Department of Physics, Auburn University, Auburn, Alabama 36849, USA — ⁵J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA

During the last 15 years a novel decay mechanism of excited atoms has been discovered and investigated. This so called "Interatomic Coulombic Decay" (ICD) involves the chemical environment of the electronically excited atom or molecule: the excitation energy is transferred to a neighbor of the initially excited particle usually ionizing that neighbor. It turned out that ICD is a very common decay route in nature as it occurs across van der Waals and hydrogen bonds. The time evolution of ICD is predicted to be highly complex, as its efficiency strongly depends on the distance of the atoms involved and this distance typically changes during the decay. Here we present a direct measurement of the temporal evolution of ICD using a novel experimental approach.

MO 5.4 Mon 17:00 C/Foyer

Enantiomeric excess determination of Chiral Molecules from Multiphoton Ionization with Femtosecond Laser Pulses — CHRISTIAN LUX, ●STEFANIE ZÜLLIGHOVEN, ALEXANDER KASTNER, TOM RING, CRISTIAN SARPE, ARNE SENFTLEBEN, and THOMAS BAUMERT — University of Kassel, Institute of Physics and CINSaT, D-34132 Kassel, Germany

Photoelectron Circular Dichroism (PECD) shows asymmetries in the electron emission from chiral enantiomers relative to the light propagation direction and was so far investigated using synchrotron radiation [1]. The magnitude of PECD is several orders larger than typically chiroptical asymmetries. We have demonstrated that PECD on randomly oriented chiral enantiomers is accessible via a 2+1 REMPI (Resonance Enhanced Multi-Photon Ionization) using femtosecond laser pulses. We detected highly structured asymmetries in the $\pm 10\%$ regime [2]. In this contribution we present our recent findings on the bicyclic Ketones Camphor, Norcamphor and Fenchone [3]. From the results on variation of the laser intensity, we conclude an underlying dissociative ionization. A quantification of different enantiomeric mixtures reveals the sensitivity of the PECD to the enantiomeric excess. The enantiomeric excess in mixtures of R- and S-Fenchone can be distinguished in the 1% regime.

[1] I. Powis Adv. Chem. Phys. 138, 267-329 (2008)

[2] C. Lux et al., Angew. Chem. Int. Ed. 51, 5001-5005 (2012)

[3] C. Lux et al., ChemPhysChem, DOI: 10.1002/cphc.201402643 (2015)

MO 5.5 Mon 17:00 C/Foyer

Extended quantum jump description of vibronic two-dimensional spectroscopy — ●JULIAN ALBERT, MARTIN KESS, MIRJAM FALGE, JOHANNES G. WEHNER, and VOLKER ENGEL — Institut für Physikalische und Theoretische Chemie, Emil-Fischer-Str. 42, Universität Würzburg, 97074 Würzburg, Germany

We calculated two-dimensional vibronic spectra for model systems involving two electronic molecular states. The coupling to a bath is simulated using a quantum-jump approach. For the latter, we use a method introduced by Makarov and Metiu [1] which includes an explicit treatment of dephasing. In this way it is possible to characterize the influence of dissipation and dephasing on the 2D-spectra.

[1] D. E. Makarov and H. Metiu, J. Chem. Phys. 111, 10126 (1999).

MO 5.6 Mon 17:00 C/Foyer

Acceleration of Singlet Fission in an Aza-Derivative of TIPS-Pentacene — ●JULIA HERZ¹, FABIAN PAULUS², JENS ENGELHART², TIAGO BUCKUP¹, UWE BUNZ², and MARCUS MOTZKUS¹ — ¹Physikalisch-Chemisches Institut — ²Organisch-Chemisches Institut, Ruprecht-Karls-Universität, D-69120 Heidelberg, Germany

Singlet fission plays a prominent role in raising the quantum efficiency of organic solar cells. In this overall spin-conserved process two molecules in the triplet state T1 are formed by investing just one photon. Pentacene is known to undergo singlet fission and is an attractive starting compound to develop new chromophores with promising photo-physico-chemical qualities. By means of ultrafast transient absorption measurements with high time resolution, we provide a detailed picture of the excited state dynamics of TIPS-pentacene [1], an important, soluble derivative of pentacene. A kinetic model was derived by carrying out a global target analysis. Furthermore, we found that a carbon to nitrogen substitution has a high impact on the triplet formation and leads to faster initial dynamics. The chemical modification can accelerate singlet fission in the aza-derivative by almost a factor of two. A faster relaxation from the singlet to triplet manifold implies a higher efficiency, because other relaxation channels are avoided. A stronger triplet signal in the near infrared spectral region relative to that in the visible indicates a higher quantum yield when compared to TIPS-pentacene, making the more air-stable aza-derivatives promising for organic electronics applications. [1] Herz et al, JPC Let. 5 (2014) 2425.

MO 5.7 Mon 17:00 C/Foyer

Optimization of the measurement method of fs pump-probe experiment by compressed sensing — ●DANIEL UHL, LUKAS BRUDER, MARCEL BINZ, MARCEL MUDRICH, AARON LAForge, DAVID GROSS, and FRANK STIENKEMEIER — Physikalisches Institut,

Universität Freiburg, Germany

Deducing the spectrum of a fs spectroscopy experiment generally requires sampling the signal in the time domain at a rate that suffices the Shannon-Nyquist-Theorem. This boundary condition can result in very long acquisition times especially in multi-dimensional spectroscopy setups where even more data points are required. Compressed sensing reconstructs a signal by exploiting the sparsity of the signal in the frequency domain and allows for sampling far below the Shannon-Nyquist-Theorem in the time domain, while yielding the same information content. In view of combining this method with 2D spectroscopy we are investigating at first its applicability to fs pump-probe spectroscopy. We have investigated quantum beat spectra of atomic vapors and a simple diatomic molecule by analyzing simulated as well as experimental data with this method.

MO 5.8 Mon 17:00 C/Foyer

Realization of Ultrafast Logic Gate for Reversible Computation by Nonlinear Optical Techniques — ●MEHDI MOHAMMAD KAZEMI, ALIREZA MAZEHERI TEHRANI, TAHIR ZEB KHAN, and ARNULF MATERNY — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

A Toffoli gate (CCNOT gate) is a universal reversible logic gate, from which all other reversible gates can be constructed. It has a three-bit input and output. The goal of our work was to realize a Toffoli gate where all inputs and outputs are realized optically, which allows for ultrafast switching processes. We demonstrate experimentally that a Toffoli logic gate can be based on nonlinear multi-wave interactions of light with matter. Using femtosecond laser pulses, the all-optical Toffoli gate is making use of the coherence of the optical signal produced via the nonlinear optical process. Sum frequency (SF) and second harmonic (SH) generations are combined in such a way so as to yield the complete truth table of the universal reversible logic gate.

MO 5.9 Mon 17:00 C/Foyer

Time-dependent photoelectron spectroscopy of all-trans retinal in liquid micro-jet — ●LASON KATECHIS¹, KATHRIN AZIZ-LANGE^{1,2}, MARTIN ECKSTEIN¹, JOHAN HUMMERT¹, FRANZISKA BUCHNER¹, ANDREA LÜBCKE¹, and OLEG KORNILOV¹ — ¹Max Born Institute Berlin, Germany — ²present address: Helmholtz Zentrum Berlin, Germany

The isomerization of all-trans-retinal, the primary step in vision, has been studied in great detail. Nevertheless the ordering of its excited states, their lifetimes and how these are affected by different solvent environments remain unclear. Time-resolved femtosecond spectroscopy promises to shed light on these questions, however several studies performed so far report contradictory results on the lifetimes observed in experiments and this leads to an ambiguity in the choice of a photophysical model.

In our study we employ time-resolved photoelectron spectroscopy of retinal in a liquid micro-jet for different solvents. We observe that it is important to investigate different data analysis strategies since they can lead to contradicting results. We hence compare methods including global fitting and singular value decomposition (SVD) along with more flexible photophysical models than those assumed so far in order to get deeper insight into the underlying mechanisms.

MO 5.10 Mon 17:00 C/Foyer

Coherent and incoherent contributions to the carrier-envelope phase control of wave packet localization in quantum double wells — ●KILIAN HADER — Institut für Physikalische und Theoretische Chemie, Emil-Fischer-Str. 42, Universität Würzburg, 97074 Würzburg, Germany

We study laser excitation processes in a double well potential. The possibility to influence localization via the carrier-envelope phase (CEP) of a laser pulse is investigated for various situations which differ in the nature of the initial state prior to the laser interactions. In more detail, the CEP-dependence of asymmetries in the case where initially the system is described by localized wave packets, eigenstates or incoherent mixtures are calculated and interpreted within time-dependent perturbation theory. It is investigated which contributions to the asymmetry exist and how they can be modified to reveal a more or less pronounced CEP-effect.

[1] K. Hader, V. Engel, J. Chem. Phys. 140, 184316 (2014)

MO 5.11 Mon 17:00 C/Foyer

Dissociative electron attachment in biologically relevant

molecules — ●MARVIN WEYLAND^{1,2}, ALEXANDER DORN², HANS RABUS¹, XUEGUANG REN^{1,2}, THOMAS PFLÜGER^{1,2}, and WOON YONG BAEK¹ — ¹Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — ²Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany

Dissociative electron attachment (DEA) is presumed to be a large contributor to radiation damage in biological tissue and, therefore, has gained increased attention during the last decade. We set up a COLTRIMS-type instrument, adapted for negative ion detection to measure emission angles and energies of anions created in DEA-processes. Using a photoemission electron source we reach an impact energy resolution of 200 meV at about 1 μ A peak current, thereby improving energy resolution compared to previous setups. First experiments have been performed with ammonia, investigating DEA in the monomer and small clusters. Advancing towards biologically relevant molecules we investigated furan. This liquid target is introduced using a seeded supersonic gas jet. We studied several fragmentation products at the DEA resonance around 6 eV electron impact energy, which should allow a more detailed understanding of the attachment process.

MO 5.12 Mon 17:00 C/Foyer

Dipole-driven dynamics for near threshold electron/positron interactions with DNA/RNA bases — ●FABIO CARELLI¹, JAN FRANZ², and FRANCO A. GIANTURCO^{1,3} — ¹Institute for Ion Physics and Applied Physics, Innsbruck University, 6020 Innsbruck, Austria — ²Department of Atomic, Molecular and Optical Physics, University of Technology, 80-233 Gdansk, Poland — ³Scuola Normale Superiore, 56125 Pisa, Italy

It is well known that when an external ionizing radiation interacts with living organisms, one of the mechanisms responsible for genetic damage involves metastable attachment of secondary low-energy electrons to DNA/RNA bases, while the interactions of low-energy positrons in molecular biological gases or in condensed media has found a wide-spread range of applications (for example the role of positronium formation/annihilation probabilities in different environments).

For all the above processes, the knowledge of the paths by which the impinging lepton attaches biomolecules is crucial.

We know that for gas-phase rotating polar molecules with supercritical dipoles a finite number of Rydberg-like states involving e^- exists (and for e^+ could exist, being mainly differentiated by the spatial orientation).

The interaction dynamics of DNA/RNA bases (all having large permanent dipoles) with near-threshold collisions involving e^-/e^+ shall be presented and discussed: the aim is suggesting a new formation/stabilization mechanism for charged biomolecules occurring through a more 'gentle' energy release path.

MO 5.13 Mon 17:00 C/Foyer

Cryo spectroscopy of size selected cobalt clusters — ●SEBASTIAN DILLINGER, JENNIFER MOHRBACH, MAXIMILIAN GAFFGA, JOACHIM HEWER, and GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

We have performed Infrared (Multiple) Photon Dissociation (IR(M)PD) spectroscopy of adsorbed nitrogen on size selected cobalt cluster cations (Co_n^+ , $n = 8 - 17$) at well-defined cryo temperatures. Our setup combines a hexapole ion trap for kinetic studies with a FT-ICR cell for IR(M)PD studies and mass analysis. Both ion traps are cryogenically cooled to temperatures below 30 K. The cold IR(M)PD spectra of the $[\text{Co}_n(\text{N}_2)_1]^+$ clusters reveal well resolved bands. All complexes show single or multiple IR active bands within the range of 2180 to 2290 cm^{-1} (2110 - 2350 cm^{-1} probed). These bands are significantly red shifted with respect to the IR inactive stretching mode of free N_2 (at 2359 cm^{-1}). Preliminary ab initio DFT calculations augment the current experiments, failing to provide unambiguous structural conclusions as of now.

MO 5.14 Mon 17:00 C/Foyer

Theoretical description of ultra-long-range Rydberg molecules — ●CHRISTIAN FEY¹, MARKUS KURZ¹, and PETER SCHMELCHER^{1,2} — ¹Zentrum für optische Quantentechnologien, Universität Hamburg — ²Hamburg Centre for Ultrafast Imaging, Universität Hamburg

Ultra-long-range Rydberg molecules are "giant molecules" that consist of a Rydberg atom whose valence electron bounds one or even more

ground state atoms by partial wave scattering at equilibrium distances of several 1000 Å. They differ from usual molecules not only by their exotic physical properties (e.g. dipole moments $\sim 10^3$ Debye) but also by their theoretical description. Here we review and link the different theoretical methods which are currently employed in the literature to determine the molecular Born-Oppenheimer potential curves. These methods rely either on zero-range Fermi-like pseudopotentials (e.g. bare or regularized delta potentials) or on the use of the Coulomb Green's function inside quantum defect theory.

MO 5.15 Mon 17:00 C/Foyer

Motion manipulation of 4-aminobenzonitrile with microwave fields — ●JACK GRANEEK, SIMON MERZ, THOMAS BETZ, and MELANIE SCHNELL — Max-Planck-Institut für Struktur und Dynamik der Materie at the Center for Free-Electron Laser Science, 22761 Hamburg, Germany

To manipulate the motion of large and complex molecules, or molecules in their ground state it is necessary to employ methods that are compatible with high-field-seeking states. High-field-seeking states are attracted to field maxima, which cannot be realized in free space with static fields. Therefore, motion manipulation of such states requires the use of time-dependent fields. A previous experiment using microwave fields within a resonator achieved an additional deceleration of a pre-decelerated packet of ammonia molecules [1]. Here, we employ a modified experimental setup for the manipulation of a molecular beam of 4-aminobenzonitrile (ABN), a larger and heavier (118 g/mol) molecule, directly from a supersonic expansion. ABN displays a large dipole moment. It is an asymmetric top so also has a more complex rotational structure. In order to predict the AC Stark shift of the ABN rotational levels within our microwave resonator we have developed a numeric simulation. From this we can determine which rotational states are more accessible for focusing with a microwave lens. Here, we will present the results of calculations carried out as well as details on the new experimental set up.

[1] S. Merz, C. Brieger, N. Vanhaecke, G. Meijer, and M. Schnell, *Mol. Phys.* 111, 1855-1864 (2013).

MO 5.16 Mon 17:00 C/Foyer

Evidence for long-lived collision complexes in scattering of ultracold ground-state molecules — ●KATHARINA LAUBER, EMIL KIRILOV, MANFRED MARK, FLORIAN MEINERT, and HANNS-CHRISTOPH NÄGERL — Institut für Experimentalphysik, Universität Innsbruck, 6020 Innsbruck, Österreich

Ultracold molecules trapped in optical lattice potentials at high densities and prepared in their lowest internal quantum state are an ideal starting point for fundamental studies in physics and chemistry, ranging from novel quantum gas experiments and cold controlled chemistry to quantum simulation. We create ultracold and dense samples of Cs dimer molecules in their rovibrational ground state in an optical lattice with near unity occupation probability at the individual lattice sites. The preparation involves the formation of a Cs Bose-Einstein condensate, the transition to a Mott-insulating state, the formation of Feshbach molecules, and coherent 4-photon ground-state transfer. Lowering the lattice potential along one or two directions allows us to probe the molecules' collisional properties in one- and two-dimensional geometry, respectively. Atoms can also be used as scattering partners. In all cases under investigation we observe rather rapid loss of molecules, in particular when the molecules are in their absolute hyperfine ground state. We attribute such loss to the formation of elastically bound long-lived collision complexes, i.e. the formation of atom-dimer or dimer-dimer two-body complexes, which then undergo a secondary collision with another atom or molecule. We model our data to derive rate coefficients and lifetimes and compare the results to recent predictions.

MO 5.17 Mon 17:00 C/Foyer

A High Resolution Microwave Spectrometer to Study Large Chiral Molecules — ●CHRIS MEDCRAFT^{1,2}, ROBERT WOLF³, and MELANIE SCHNELL^{1,2} — ¹Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — ²Center for Free-Electron Laser Science, Hamburg, Germany — ³Universität Regensburg, Institut für Anorganische Chemie, Regensburg, Germany

A high-resolution, cavity-based Fourier-transform microwave spectrometer is being commissioned in Hamburg. The spectrometer is based around the COBRA design (Coaxially Oriented Beam-Resonator Arrangement^[1]). The higher resolution (ca. 3 kHz) and larger spectral range (6-40 GHz) of this instrument will complement our broad-

band chirped-pulse FTMW spectrometer^[2] (2-8.5 GHz), allowing for investigations of nuclear quadrupole hyperfine structure and internal rotation. When combined with a source of cold, slow molecules,^[3] transit-time and Doppler broadening is reduced and the enhanced resolution may be able to discriminate the parity violating effects in large chiral molecules such as CpRe(NO)(CO)I (Cp=cyclopentadienyl). The rotational spectrum of the related molecule CpRe(CH₃)(CO)(NO) has been measured using the chirped-pulse FTMW spectrometer showing that the analysis of such large and complicated molecules is feasible.^[4]

[1] Grabow, *Rev. Sci. Instrum.*, 67, 4072 (1996)

[2] Schmitz, Shubert, Betz, Schnell, *J. Mol. Spec* 280 (2012) 77

[3] Merz, Vanhaecke, Jäger, Schnell, Meijer, *Phys. Rev. A* 85, (2012) 063411

[4] Medcraft, Wolf, Schnell *Angew. Chem. Int. Ed.* 53 (2014) 11656

MO 5.18 Mon 17:00 C/Foyer

Infrared Spectroscopy of Helium Solvated π -conjugated Organic Radicals — ●DANIEL LEICHT, DANIEL HABIG, MATIN KAUFMANN, GERHARD SCHWAAB, and MARTINA HAVENITH — Physikalische Chemie II, Ruhr-Universität Bochum

Helium nanodroplet infrared spectroscopy is a well established experimental technique to study weakly bound complexes as well as reactive species. [1] Superfluid helium hardly interacts with the embedded species, which leads to only small matrix-induced shifts. Recently, different reactive molecules (e.g. organic radicals) have been studied using helium nanodroplet spectroscopy. [2,3] In this work we present some of our latest results regarding π -conjugated radicals. Examples are allyl, benzyl and cyclopentadienyl radicals that are important intermediates in many reactions in e.g. combustion, explosives and in tropospheric chemistry. Apart from studying the bare radical also aggregates with other molecules (e.g. allyl radical + HCl) and reactions at cold temperatures (e.g. allyl radical + NO [2]) can be investigated using our technique.

[1] M. Choi, G. Douberly, T. Falconer, W. Lewis, C. Lindsay, J. Merritt, P. Stiles and R. Miller, *International Reviews in Physical Chemistry*, 2006, 25, 15-75

[2] D. Habig, D. Leicht, M. Kaufmann, G. Schwaab, M. Havenith, *The Journal of Chemical Physics*, 141, 044312 (2014)

[3] Jochen Küpper, Jeremy M. Merritt, *International Reviews in Physical Chemistry*, 26, Iss. 2, 2007

MO 5.19 Mon 17:00 C/Foyer

Precise FTIR Study of Ethylene and Its Isotopomers — OLEG N. ULENIKOV¹, OLGA V. GROMOVA¹, ELENA S. BEKHTEREVA¹, KARL-HEINZ GERICKE², CHRISTOF MAUL², and ●SIGURD BAUERCKER² — ¹Department of General Physics, Tomsk Polytechnic University, Russia — ²Institut für Physikalische und Theoretische Chemie, TU Braunschweig, Germany

Ethylene is one of the most relevant substances in the study of numerous both pure scientific and applied problems of physics, chemistry, and astrophysics. Ethylene plays an important role in structural chemistry. In particular, its C=C bond length has been chosen as a standard in the discussion of molecular structure. The present work is part of a systematic analysis of the spectra of ethylene and its isotopomers. We report recent results of high resolution studies of the 12C₂H₄, 13C₂H₄, 12C₂H₃D, 12C₂H₂D₂-trans, 12C₂H₂D₂-cis, and 12C₂H₂D₂-as ethylene isotopic species. Precise infrared spectra were measured with a FTIR spectrometer Bruker 120HR at different temperatures, pressures and path lengths. Spectra have been recorded in the region of the 1200-6000 cm⁻¹. Transitions in all the recorded spectra have been assigned and further analysis was made in the frame of the model which takes into account numerous resonance interactions in the sets of bands located in the corresponding spectral regions. The obtained sets of spectroscopic parameters allow to use the obtained information both for a further precise analysis of the line strengths and shape of spectral lines of ethylene and its isotopomers, and also for a correct determination of the ethylene intramolecular potential energy surface.

MO 5.20 Mon 17:00 C/Foyer

Temporal characterization studies of an ultrafast electron diffractometer — ●XAVIER HOLZAPFEL, CHRISTIAN GERBIG, SILVIO MORGENSTERN, MARLENE ADRIAN, ARNE SENFTLEBEN, and THOMAS BAUMERT — University of Kassel, Institute of Physics and Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

Time-resolved diffraction, using x-ray or electron probes, has become a promising technique to directly provide insights into dynamics at

the molecular level with ultrafast precision. We study the dynamical processes in single crystalline graphite by means of ultrafast electron diffraction in order to expand the understanding of phonon generation and decay mechanisms being essential for future carbon based electronic devices. Our highly compact DC electron diffractometer is fully characterized by experiments and N-body simulations. At balanced conditions a temporal resolution of 200 fs along with high-definition diffraction is achieved for dynamical studies.

In this contribution the temporal characterization of electron pulses is discussed in dependency of different characterization methods. We use grating enhanced ponderomotive scattering and also electron pulse autocorrelation to characterize electron pulses in situ.

MO 5.21 Mon 17:00 C/Foyer

Improving the Angular Accuracy in Molecular Beam-Surface Scattering Experiments — •PAUL SAFTIEN, BO-GAUN CHEN, and WOLFGANG CHRISTEN — Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 2, 12489 Berlin, <http://clusterlab.de>

In molecular beam-surface scattering experiments a precise alignment of the incoming beam, the target surface, and the particle detector is desirable.

We present a straightforward method allowing for an accurate positioning of the solid substrate in molecular beam-surface scattering experiments such that the beam-surface-detector angle is well defined. The method is demonstrated for measurements of the angular distribution of a pulsed supersonic helium beam, scattered off a chemically inert Si(111)/SiO₂ surface. Based on a geometric model, target and detector positions are systematically varied in order to obtain a most precise surface alignment.

MO 5.22 Mon 17:00 C/Foyer

Laser-induced acoustic desorption of large molecules — •ZHIPENG HUANG^{1,3}, DANIEL A. HORKE¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY, Hamburg — ²Center for Ultrafast Imaging, University of Hamburg — ³Department of Physics, University of Hamburg

State-, conformer-, and size-selection of small neutral molecules can be achieved through the dispersion of the molecular beam with electric fields [1]. State-selected small molecules can then be well aligned and oriented by laser and static electric fields [2]. To extend these techniques to large molecules is currently limited by the ability to produce

high densities of neutral large molecules in the gas-phase.

Laser-induced acoustic desorption (LIAD) is a promising technique for gentle and efficient preparation of intact neutral large molecules in vacuum. Here we demonstrate our newly set-up laser-induced acoustic desorption (LIAD) source, which is coupled to a time-of-flight mass spectrometer. We will discuss the efficiency of the source as a function of experimental parameters, such as laser pulse energy, duration and foil parameters, and discuss its potential for applications in x-ray or electron diffraction imaging.

[1] S. Y. T. van de Meerakker et al., *Chem. Rev.* **112**, 4828 (2009); Y.P. Chang et al., *Science* **342**, 98 (2013); T. Kierspel et al., *Chem. Phys. Lett.* **591**, 130 (2014); D. Horke et al., *Angew. Chem. Int. Ed.* **53**, 11965 (2014)

[2] H. Stapelfeldt et al., *Rev. Mod. Phys.* **75**, 543 (2003); S. Trippel et al., *Phys. Rev. A* **89**, 051401(R) (2014); arXiv:1409.2836

MO 5.23 Mon 17:00 C/Foyer

Investigation on Citrus Oils Using Raman Spectroscopy with Different Excitation Wavelengths — •KATERINA KANEVCHE, RASHA HASSANEIN, BERND VON DER KAMMER, and ARNULF MATERNY — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

Citrus oils are essence oils manufactured from various citrus fruits. Major constituents include *e.g.* limonene and other terpenes. Carotenoids, only found in minor quantities, present key organic pigments absorbing in the visible (VIS) range between 400 and 550 nm, thus protecting the chlorophyll deterioration due to sun-light exposure. Moreover, they act as antioxidants in the human body. Limonene and citral are mainly responsible for the odor of citrus fruits. They are used in manufacturing cosmetic products as well as food flavors, perfumes, etc. Both carotenoids and carbohydrate terpenes can be identified from their Raman spectrum. Earlier experiments have applied FT-Raman to citrus oils. Here, we introduce Raman spectroscopy using different wavelengths in the VIS spectral range for the investigation of oils from various citrus fruits. Detailed vibrational information could be obtained much faster and resonance Raman effects could be used giving access to minor species. Chemometric analysis has been employed in order to discriminate between the different oils based on their composition. VIS Raman spectroscopy thus constitutes a fast, non-destructive analytical technique not requiring sample preparation, which would be a very attractive tool for inline monitoring of the production process and quality control of citrus oils.