A 18: Interaction with strong or short laser pulses II

Time: Tuesday 14:00–16:00 Location: BEBEL E34

Invited Talk A 18.1 Tue 14:00 BEBEL E34

Determination of chiral molecules' handedness — •Markus Schöffler[1], Martin Pitzer[1], Maksim Kunitski[1], Allan S. Johnson[1,2], Till Jahnke[1], Hendrik Sann[1], Felix Sturm[1], Lothar Ph. H. Schmidt[1], Horst Schmidt-Böcking[1], Reinhard Dörner[1], Jürgen Stohner[3], Julia Kiedrowski[4], Michael Reggelin[4], Sebastian Marquardt[4], Alexander Schiesser[4], and Robert Berger[4] — [1]Institut für Kernphysik, J. W. Goethe-Universität Frankfurt, Germany — [2]University of Ottawa, ON K1N 6N5, Canada — [3]Institute of Chemistry and Biological Chemistry, Zurich, 8820 Wädenswil, Switzerland — [4]Clemens-Schöpf Institute, TU Darmstadt, Germany

When reaching a certain level of complexity, molecules can have a chiral structure. This is similar to our hands, which also exist in a right and a left version. As the molecules have the same physical properties (density, melting point etc.) determination of the two species poses major challenges even today to chemists. Many indirect methods have been developed therefore with more or less drawbacks. An intense femtosecond laser pulse was used to remove many electrons (>4) from the molecule, resulting in a Coloumb Explosion of the molecules fragments. The COLTRIMS momentum imaging technology COLTRIMS was employed to measure the momentum vector of each emitted fragment (ion and electron) in coincidence. The show case example of racemic CHBrClF will be presented, the fragmentation dynamics discussed and the chiral distinction illustrated. Furthermore the perspectives on larger molecules will be discussed, as well as the challenges using synchrotron radiation

A 18.2 Tue 14:30 BEBEL E34

Photoelectron circular dichroism in above threshold ionization of chiral molecules — •Ingo Dreissigacker and Manfred Lein — Institut für Theoretische Physik, Leibniz Universität Hannover

Motivated by a recent experiment on circular dichroism in the photoelectron momentum distributions of chiral molecules from strong-field ionization [Lux et al., Angew. Chem. Int. Ed. 51, 5001 (2012)], we investigate this effect theoretically. For the first time, we are able to compute the asymmetric response of a sample of randomly oriented chiral molecules to a strong circularly polarized field non-perturbatively and from first principles. The strong-field approximation fails to describe this process due to its plane-wave nature. We therefore apply the Born approximation to the scattering state and use this as a continuum-state correction in the strong-field approximation. In this way, we obtain spectra of the molecules camphor and fenchone and study contributions of individual molecular orientations to the asymmetric photoelectron emission in order to improve the physical understanding of the process.

A 18.3 Tue 14:45 BEBEL E34

Controlling the strong-field dissociation of aligned C_2H_2 ions — •Katharina Doblhoff-Dier[1,2], Xinhua Xie[2], Markus Kitzler[2], and Stefanie Gräfe[1] — [1]Friedrich Schiller Universität, Jena, Deutschland — [2]Technische Universität Wien, Wien, Österreich

Intense, short near infra-red laser sources provide novel tools to control molecular reactions, e.g., via the CE phase[1]. Recently, experimental results have shown the possibility to control fragmentation reactions in acetylene by aligning the molecule relative to the laser polarization direction. In our work, we use these results to gain a better insight into the underlying mechanisms and to obtain an interpretation of the rich experimental results. Simplifying the complex, quantum mechanical dissociation process, we discompose the reaction into several interconnected steps, allowing for their separate modelling and analysis. The complexity of the process, however, requires a wealth of different models. Amongst others, we apply time-dependent density functional theory, molecular tunnelling theory, single orbital electron impact ionization, reduced dimensional quantum dynamics calculations modelling field excitation processes, and both quantum mechanical and (semi-)classical estimates. The comparison and synopsis of all sub-processes allows us to confirm and identify not only multi-orbital contributions but also to investigate the influence of different ionization mechanisms (sequential and non-sequential), relevant for the dissociation process. We hope that the classification of different processes will also help to understand laser aided reactions in more complex molecules.

[1] Xie et al., Phys. Rev. Lett. 109, 243001 (2012)

A 18.4 Tue 15:00 BEBEL E34

Exact TDSE simulations of H_2^+ in intense laser fields — •Volker Mosert and Dieter Bauer — Institut für Physik, Universität Rostock, 18051 Rostock

We investigate ionization of the hydrogen molecular ion H_2^+ in intense laser fields, in particular the influence of the nuclear motion beyond Ehrenfest dynamics. Simulating molecules in intense laser fields on an *ab initio*-level is in general prohibitive because the time dependent Schrödinger equation (TDSE) for electrons *and* ions has to be solved. However, the problem of H_2^+ in a laser field polarized colinear to the internuclear distance can be reduced to three dimensions when the cylindrical symmetry is exploited. We discretize the problem on a non-equidistant cylindrical grid. A finite difference approximation of the Hamiltonian in conjunction with a Crank-Nicolson time propagator is used to solve the TDSE.

A 18.5 Tue 15:15 BEBEL E34

Multi-channel ionization dynamics of finite systems under intense Xray pulses — •Abraham Camacho Garibay, Ulf Saalmann, and Jan-Michael Rost — MPI-PKS

Xray free-electron lasers sources provide ultra-intense and ultra-short pulses, allowing the study entirely new regimes of light-matter interaction. In particular, a cluster or molecule can absorb many photons, creating a deep Coulombic potential, which depends on the instantaneous charge and instantaneous size of the (expanding) system. This potential modifies energies of photo- and Auger electrons in a characteristic manner. By means of the measurable electron spectra one may uncover the complex electron and ion dynamics in the cluster or molecule.

A 18.6 Tue 15:30 BEBEL E34

Quantum trajectory analysis of clusters and molecules in strong laser fields — •Thomas Keil and Dieter Bauer — Universität Rostock, Institut für Physik

The strong field approximation (SFA) is *the* underlying theory describing the interaction of intense laser light with atoms or molecules. However, it has been noted that several spectral features are not reproduced by the plain SFA because the Coulomb force on the outgoing photoelectron is neglected. It is well-known that photoelectrons generated by strong-field ionization of atoms have a cut-off energy of $2U_p$ if they move directly to the detector (or $10U_p$ if they rescatter once from their parent ion). Electrons emitted from laser-irradiated clusters may have much higher kinetic energies, especially at resonance [1,2]. We apply the methodology developed for the Coulomb-corrected SFA (CCSFA) based on quantum trajectories [3] to a SFA that is corrected for the collective electric field in the cluster. We show that it is this collective field, which arises because of the coherent oscillation of the electron cloud with respect to the ionic background, that generates multi-U_p electrons. This finding comfirms the "surface-plasmon-assisted rescattering in clusters" revealed earlier via classical molecular dynamics simulations [1]. Results from the CCSFA for molecules will be also presented.

[1] Th. Fennel et al., Phys. Rev. Lett. 98, 143401 (2007).
[2] Th. Keil, D. Bauer, J. Phys. B (submitted).
[3] T.-M. Yan et al., Phys. Rev. Lett. 105, 253002 (2010); T.-M. Yan et al., Springer Series in Chemical Physics vol. 104 (2013).

A 18.7 Tue 15:45 BEBEL E34

Field-driven THz-streaking of Nanotip Photoemission — •Georg Herink, Lara Wimmer, Katharina E. Echternkamp, Daniel R. Solli, and Claus Ropers — 4. Physical Institute - University of Göttingen, Göttingen, Germany

We present an ultrafast, nanoscale streaking scheme for field-driven photoemission control using single-cycle THz transients at the apex of a sharp gold tip [1]. The locally enhanced THz-field allows for a high-contrast enhancement or suppression of the near-infrared photoemission yield and a tuning of the photoelectron kinetic energy distribution, both in spectral position and width.

This streaking scheme is unique to nanostructures because of the strong sub-wavelength confinement of the driving field [2]. In particu-

lar, the associated electron dynamics are governed by the momentary THz field at the instance of photoemission, rather than by a temporal integral, i.e. the vector potential, as in optical streaking experiments for attosecond spectroscopy [3].

Besides the fundamental interest in the characterization and control of electron trajectories within ultrashort optical near-fields, the approach carries significant potential for pulse compression in ultrafast electron diffraction and microscopy experiments.

[1] Wimmer et al., arXiv: 1307:2581 (2013)
[2] Herink et al., Nature 483, 190-193 (2012)
[3] Corkum, Krausz, Nature Physics 3, 381 - 387 (2007)