

## INTENSE FIELD INTERACTION WITH MOLECULES AND CLUSTERS (SYIF)

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**ÜBERSICHT DER HAUPTVORTRÄGE UND FACHSITZUNGEN**  
 (Hörsaal HV)

SYIF 1.1 Fr 14:00 (HV) Introduction, Ingolf Hertel

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SYIF 1.2 Fr 14:08 (HV) **Maria Goeppert Mayer: Nobel Prize Woman in Science**, Sharon Bertsch McGrayne

SYIF 1.3 Fr 14:36 (HV) **Multiphoton photonics and applications in ultrafast chemical spectroscopies**, Margaret Murnane, Nick Wagner, Andrea Wuest, Ivan Christov, Henry Kapteyn

SYIF 1.4 Fr 15:04 (HV) **Fragmentation of molecules in intense laser fields: imaging of ultrafast molecular dynamics with coincident momentum spectroscopy**, Artem A. Rudenko, Th. Ergler, B. Feuerstein, K. Zrost, C.D. Schroeter, R. Moshammer, J. Ullrich

SYIF 1.5 Fr 15:32 (HV) **Atomic clusters in strong laser pulses: Energy spectra of emitted ions and electrons**, Ulf Saalmann

SYIF 2.1 Fr 16:30 (HV) **Applications of Attosecond Lasers to Atoms and Molecules in Strong Laser Fields**, Marc Vrakking

SYIF 2.2 Fr 17:00 (HV) **Excited state dynamics of nanostructures and biomolecules within TDDFT**, Angel Rubio

SYIF 2.3 Fr 17:30 (HV) **Strong dual-pulse excitations of metal clusters**, Karl-Heinz Meiwes-Broer, Tilo Doeppner, Thomas Fennel, Johannes Passig, Josef Tiggesbaeumker

SYIF 2.4 Fr 18:00 (HV) **New Perspectives Arising from Femtosecond Plasma Channels in Air**, Ludger Woeste

**Fachsitzungen**

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# Fachsitzungen

– Hauptvorträge –

## SYIF 1 Intense field interaction with molecules and clusters 1

Zeit: Freitag 14:00–16:00

Raum: HV

SYIF 1.1 Fr 14:00 HV

**Introduction** — ●INGOLF HERTEL — Max-Born-Institut, Max-Born-Str. 2 A, 12489 Berlin

### Hauptvortrag

SYIF 1.2 Fr 14:08 HV

**Maria Goeppert Mayer: Nobel Prize Woman in Science** — ●SHARON BERTSCH MCGRAYNE — Seattle, WA

Maria Goeppert Mayer, who shared the Nobel Prize in physics with Hans Jensen, was born and educated in Göttingen. There she fell in love with an American student. After their marriage, she moved with him to the United States in 1929 to have a career. Because of laws and university regulations against married women scientists, Maria Mayer worked at three major American universities as a volunteer faculty member without pay. She discovered the shell model of the nucleus as a volunteer professor at the University of Chicago, where she was a colleague of Enrico Fermi. She was not paid for her university research until ten years after her famous discovery. Letters from Jensen to Maria Mayer reveal their close friendship.

### Hauptvortrag

SYIF 1.3 Fr 14:36 HV

**Multiphoton photonics and applications in ultrafast chemical spectroscopies** — ●MARGARET MURNANE, NICK WAGNER, ANDREA WUEST, IVAN CHRISTOV, and HENRY KAPTEYN — Department of Physics and JILA, and NSF Engineering Research Center in Extreme-Ultraviolet Science and Technology, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309-0440

Coherent beams at soft-x-ray wavelengths[1] can be generated by focusing intense femtosecond, laser pulses into a gas. This process, called high-order harmonic generation (HHG), takes nonlinear optics to an extreme. By combining together tens to hundreds of visible laser photons, high harmonic generation upshifts laser light from the visible into the ultraviolet and soft-x-ray regions, to energies in excess of 1keV. High harmonics are usually generated from noble gas atoms. Recently however, there has been great interest in using high-harmonic generation from molecules as a probe of molecular structure and dynamics. To date, HHG from rotational wavepackets has been observed, and static, tomographic, structural information has been extracted in the case of a diatomic molecule.[2,3] In this talk, I will discuss the first observation of intramolecular dynamics using electrons rescattered during the process of high harmonic generation.[4] We first excite coherent vibrations in SF<sub>6</sub> using impulsive Raman scattering with a short laser pulse. A second, more-intense laser pulse generates high-order harmonics of the fundamental laser, at wavelengths of 20-50 nm. The high-order harmonic yield is observed to oscillate, at frequencies corresponding to all the Raman-active modes of SF<sub>6</sub>, with an asymmetric breathing mode most visible. This is in contrast to conventional impulsive stimulated Raman spectroscopy where only the symmetric breathing mode of the molecule is easily observed. The data also show evidence of relaxation dynamics following impulsive excitation of the molecule. Our results indicate that high harmonic generation is a sensitive probe of vibrational dynamics and may yield more information simultaneously than conventional ultrafast spectroscopic techniques. Since the de Broglie wavelength of the recolliding electron is on the order of interatomic distances, i.e. 1.5 Å, small changes in the shape of the molecule lead to large changes in the high harmonic yield. This work therefore demonstrates a new spectroscopic technique for probing ultra-

fast internal dynamics in molecules that uniquely combines ultrafast time resolution with atomic-scale structural information.

[1] H. Kapteyn et al., "Extreme Nonlinear Optics: Coherent X-Rays from Lasers", *Physics Today*, March (2006).

[2] R. Velotta et al., "High-order harmonic generation in aligned molecules", *PRL* 8718 (2001).

[3] J. Itatani et al. Tomographic imaging of molecular orbitals. *Nature* 432, 867-871 (2004).

[4] N. Wagner et al., "Monitoring Molecular Dynamics using Coherent Electrons from High-Harmonic Generation", submitted for publication (2005).

### Hauptvortrag

SYIF 1.4 Fr 15:04 HV

**Fragmentation of molecules in intense laser fields: imaging of ultrafast molecular dynamics with coincident momentum spectroscopy** — ●ARTEM A. RUDENKO, TH. ERGLER, B. FEUERSTEIN, K. ZROST, C.D. SCHROETER, R. MOSHAMMER, and J. ULLRICH — Max-Planck-Institut fuer Kernphysik, Postfach 103980, 69029 Heidelberg

Ultrafast molecular dynamics in strong laser fields attracts continuously increasing attention since modern lasers routinely provide pulses, which match the vibrational timescale even for the fastest molecular systems. In combination with state-of-the-art few-particle detection techniques, this offers a variety of possibilities to study molecular fragmentation with unprecedented precision. Using the so-called "Reaction Microscope", an apparatus which enables coincident measurements of the full momentum vectors of charged reaction products, we study the behaviour of the simplest molecules, H<sub>2</sub> and D<sub>2</sub>, exposed to ultrashort (6-25 fs) intense laser pulses. We disentangle different fragmentation pathways, and show how they evolve when the pulse duration becomes shorter than the vibrational period. Detailed understanding of the fragmentation mechanisms allows us to map the time evolution of dissociating and bound nuclear wave packets using a pump-probe scheme and the so-called Coulomb explosion imaging. The structure of the H<sub>2</sub><sup>+</sup> (D<sub>2</sub><sup>+</sup>) vibrational wave packet, its dephasing and subsequent revivals can be observed, as well as the signatures of vibrational and rotational motion of a neutral molecule. The experimental technique was also applied to larger molecules, such as N<sub>2</sub>, CO<sub>2</sub>, Ar<sub>2</sub>.

### Hauptvortrag

SYIF 1.5 Fr 15:32 HV

**Atomic clusters in strong laser pulses: Energy spectra of emitted ions and electrons** — ●ULF SAALMANN — Max-Planck-Institut fuer Physik komplexer Systeme, Noethnitzer Str. 38 01187 Dresden

Being prototypes of atomic many-particle systems, the response of clusters to strong laser fields has been intensively investigated for the last decade. In particular the advent of femtosecond laser pulses allowed for time-resolved studies by using variable pulse lengths or pump-probe techniques.

Here, microscopic calculations based on a mixed quantum-classical description of the laser-cluster interaction are presented. They provide, along with the measurements, valuable insight into the complex many-particle dynamics and explain the very effective absorption mechanisms as well as how this renders measured energy spectra of ions, electrons or photons emitted by the cluster. Differences in the laser-induced dynamics for high-frequency pulses (as available from novel FEL machines) are discussed briefly.

## SYIF 2 Intense field interaction with molecules and clusters 2

Zeit: Freitag 16:30–18:30

Raum: HV

**Hauptvortrag**

SYIF 2.1 Fr 16:30 HV

**Applications of Attosecond Lasers to Atoms and Molecules in Strong Laser Fields** — ●MARC VRAKING — FOM Institute for Atomic and Molecular Physics, P.O. Box 41883, 1009 DB, Amsterdam, NL

In the past two decades femtosecond time-resolved experiments have allowed the observation of molecular rotations and vibrations, and of photo-induced chemical processes. However, these experiments often tell only half the story: they show the motion of atoms moving under the influence of potential energy curves that result from a time-average over the motion of all electrons in the system. The natural time-unit for this electronic motion itself is the atomic unit of time (1 a.u. = 0.024 fsec = 24 attoseconds). Real-time observation of this motion therefore requires attosecond laser techniques. Recently the production and characterization of attosecond pulses has become possible. When considering motions of electrons we may distinguish between motion that results from driving the electrons with a strong laser field and motion that results from photo-absorption in a weak laser field. In strong laser fields the electron motion can be quite intuitive. On the other hand, studies of photo-absorption in weak laser fields are extremely important, since all photo-absorption processes in nature (i.e. outside a laser laboratory) occur in this regime. In my talk I will discuss experiments aimed at observing the motion of electrons on attosecond timescales in strong laser fields in situations where we believe that this motion explains previously made observations. An interesting example is so-called dynamic molecular alignment. For a number of years we have known that exposure of molecules to intense (femtosecond) laser fields leads to alignment of the molecule along the laser polarization axis. The accepted explanation for this phenomenon is that the electric field of the laser creates an oscillatory electron motion that generates a dipole and - in combination with the laser electric field - a torque that forces the molecule into alignment. I will discuss experiments that show very direct evidence for the existence of this oscillating dipole.

**Hauptvortrag**

SYIF 2.2 Fr 17:00 HV

**Excited state dynamics of nanostructures and biomolecules within TDDFT** — ●ANGEL RUBIO — Dpto. Fisica de Materiales, Facultad de Químicas, U. Pais Vasco, San Sebastian and European Theoretical Spectroscopy Facility (ETSF) and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

We will review the recent implementations of TDDFT to study the optical absorption of biological chromophores, one-dimensional polymers and layered materials. In particular we will show the effect of electron-hole attraction in those systems. We will follow two routes: one based on solving the Bethe-Salpeter equation and the other on an orbital-dependent OEP method on top of the GW approximation for the self-energy. Virtues and deficiencies of both methods will be illustrated.

Work done in collaboration with A. Castro, M. Marques, C. Rozzi, E.K.U. Gross, L. Wirtz, A. Marini, M. Gruning, L. Wirtz and D. Varsano and supported by the NANOQUANTA network of excellence and the Humboldt Foundation under the Bessel research award (2005)

**Hauptvortrag**

SYIF 2.3 Fr 17:30 HV

**Strong dual-pulse excitations of metal clusters** — ●KARL-HEINZ MEIWES-BROER, TILO DOEPPNER, THOMAS FENNEL, JOHANNES PASSIG, and JOSEF TIGGESBAEUMKER — Institute of Physics, University of Rostock, Universitaetsplatz 3, 18051 Rostock

Atomic clusters in intense laser fields are a nice playground to study the coupling of strong radiation into matter. In particular, non-stationary plasma effects lead to pronounced dynamics in the optical response. Recent experiments have shown that excitation with optically delayed dual pulses provides a powerful way to control the coupling of the radiation to these finite systems. Both the yield of highly charged atomic ions [1] as well as the kinetic energy of emitted electrons [2] are strongly enhanced for a particular optimal delay. After the first pulse initiates the cluster expansion the delay-dependent impact of the second pulse can be studied. In this contribution we will present experimental results on the charging dynamics by use of the femtosecond dual-pulse technique. Special emphasis will be put onto the role of the laser focus. The significance of the temporal structure of the laser field is demonstrated by complementary Vlasov calculations [3] on model systems. We attribute the distinct maximum in the charging efficiency to plasmon-enhanced ionization of the expanding cluster which is supported by the simulations [1]. Applying this method to free clusters and those which are embedded in helium droplets [4] reveals a significant influence of charge transfer processes which will be discussed.

[1] T. Doeppner, Th. Fennel, Th. Diederich et al., Phys. Rev. Lett. 94:013401, 2005

[2] T. Doeppner, Th. Fennel, P. Radcliffe et al., submitted

[3] Th. Fennel, G. Bertsch and K.H. Meiwes-Broer, Eur. Phys. J. D 29:367, 2004

[4] T. Doeppner, S. Teuber, Th. Diederich et al., Eur. Phys. J. D 24:157, 2003

**Hauptvortrag**

SYIF 2.4 Fr 18:00 HV

**New Perspectives Arising from Femtosecond Plasma Channels in Air.** — ●LUDGER WOESTE — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

When powerful femtosecond laser pulses interact with air, extended plasma channels can be formed. Their extraordinary physical properties open fascinating perspectives for the investigation of the atmosphere. The emitted white-light allows - for example - to retrieve information about the atmospheric composition including trace gases. On the other hand, non-linear light emission from the aerosol allows its remote elementary analysis, which so far is not possible by other optical methods. In addition, the phenomenon of radiation-induced nucleation can be used to withdraw information about optical super-saturation, which is also an optically inaccessible parameter so far. The electrical properties of the plasma channels open besides that fascinating perspectives with regard to lightning research. In the presentation the following aspects will be discussed:

- Conventional air monitoring methods and their limits
- Principle of the femtosecond LIDAR
- Formation and propagation of plasma channels in air
- Absorption measurements on atmospheric trace gases
- Measurements of the aerosol
- Electrical properties
- Outlook