A 30: Poster: Interaction with VUV and X-ray light

Time: Wednesday 16:00–18:30 Location: Empore Lichthof

A 30.1 Wed 16:00 Empore Lichthof

Temporal Dynamics of Stimulated Emission — •Andreas Reichegger and Jörg Evers — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

We study the temporal dynamics of stimulated emission. Stimulated emission is a fundamental quantum mechanical process of light-matter interaction, which plays a key role, e.g. in the theory of Lasers. For these purposes, we use a quantum optical model, where a single-photon-pulse will interact with an excited two-level atom. We develop signatures to assess the temporal evolution of stimulated emission in this model. Possible applications for nuclear X-ray Lasers are discussed.

A 30.2 Wed 16:00 Empore Lichthof

Time-dependent theory of resonance fluorescence for ultrafast and ultraintense x rays — •Stefano M. Cavaletto[1], Christian Buth[2], Zoltán Harman[1,3], and Christoph H. Keitel[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]Argonne National Laboratory, Argonne, IL, USA — [3]ExtreMe Matter Institute (EMMI), Darmstadt, Germany

The recent development of intense sources of coherent x-ray radiation such as the Linac Coherent Light Source (LCLS) in Menlo Park, California, USA, provides one with an unprecedented way to study nonlinear physics at short wavelengths. In this regard, resonance fluorescence, i.e. the spectrum of photons scattered off atoms and molecules driven by a near-resonant electric field, is expected to play a decisive role. We compute the time-dependent spectrum of resonance fluorescence of a two-level system excited by an ultrashort pulse. We allow for inner-shell hole decay widths and destruction of the system by further photoionization. This two-level description is employed to model neon cations strongly driven by LCLS light tuned to the $1s\,2p^{-1} \rightarrow 1s^{-1}\,2p$ transition at 848 eV: x rays induce Rabi oscillations which are so fast that they compete with Ne 1s-hole decay. First, we predict resonance fluorescence spectra for chaotic pulses generated at present-day LCLS; second, we explore the exciting novel opportunities offered by Gaussian pulses which will become available in the foreseeable future with self-seeding techniques. In the latter case, we predict a clear signature of Rabi flopping in the spectrum of resonance fluorescence.

A 30.3 Wed 16:00 Empore Lichthof

THz-XUV Pump-Probe Experiment Using a REMI at FLASH — •Jakob Kunz[1], Georg Schmid[1], Kirsten Schnorr[1], Nikola Stojanovic[2], Artem Rudenko[3], Lutz Foucar[4], Arne Senftleben[1], Shaofeng Zhang[1], Thomas Pfeifer[1], Joachim Ullrich[5], Yuhai Jiang[6], Alexander Broska[1], Michael Gensch[7], Alaa Al-Shemmary[2], Matthias Kuebel[8], Claus-Dieter Schroeter[1], and Robert Moshammer[1] — [1]MPIK Heidelberg — [2]DESY Hamburg — [3]Kansas State University Manhattan — [4]ASG Hamburg — [5]PTB Braunschweig — [6]Shanghai Advanced Research Institute — [7]Hemholtz-Zentrum Dresden-Rossendorf — [8]MPQ Garching

Using a Reaction Microscope (REMI) we study the fragmentation dynamics of atoms and molecules in a pump-probe scheme with a fs XUV-pulse at 58 eV and a fully synchronized strong THz-pulse at a wavelength of 150 μm. The three dimensional momenta of all charged particles are reconstructed which allows in particular the investigation of angular distributions and energies as a function of the time delay. Streaking of ions and electrons originating from ionization of atoms and molecules is demonstrated. We map the shape of the THz pulse via emission of photoelectrons created by the XUV-pulse into the THz field. Furthermore streaking as a tool to trace atomic processes, such as Auger decay in real time is discussed.

A 30.4 Wed 16:00 Empore Lichthof

Photofragmentation of Molecular Iodine studied by VIS/XUV- and XUV/XUV-Pump-Probe Measurements at FLASH — •Georg Schmid[1], Kirsten Schnorr[1], Jakob Kunz[1], Arne Senftleben[1], Artem Rudenko[2], Thomas Pfeifer[1], Kristina Meyer[1], Theo Zouros[3], Joachim Ullrich[4], Yuhai Jiang[5], Stefan Düsterer[6], Claus-Dieter Schröter[1], and Robert Moshammer[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg — [2]Kansas State University, Manhattan — [3]University of Crete, Heraklion — [4]PTB, Braunschweig — [5]Shanghai Advanced Research Institute, Shanghai — [6]DESY, Hamburg

In a pump-probe experiment the photofragmentation of molecular iodine using an ultrashort XUV pulse at $\approx$ 14 nm delivered by the free-electron-laser facility FLASH and a femtosecond IR laser pulse at $\approx$ 800 nm was performed. In order to trace the photoionization dynamics as a function of the internuclear distance, the delay between XUV- and IR-pulse is varied. A preceding IR-pulse removes valence electrons and the I_2 molecule starts to dissociate which is then probed via the inner-shell absorption of multiple XUV photons. At 14 nm the FEL creates dominantly 4d core holes followed by Auger cascades which results in charge states up to I_2^{15+}. Thus the interplay between valence- and core-electrons as a function of time is studied. A second time resolved experiment with XUV-pump and XUV-probe allows to investigate core/core electron dynamics.With both schemes we analyze the charge-up behaviour of molecular ions and ionic fragments applying coincident detection of all ion species in a reaction microscope.

A 30.5 Wed 16:00 Empore Lichthof

Isomer depletion via photons and electrons generated by an XFEL pulse — •Jonas Gunst, Adriana Pálffy, and Christoph H. Keitel — Max-Planck Institut für Kernphysik, Heidelberg

Long-lived nuclear excited states also known as isomers can store large amounts of energy over long periods of time. Much interest arises from a number of fascinating potential applications related to the controlled release of nuclear energy on demand, such as nuclear batteries. Here we investigate the controlled depletion of the 2.4 MeV ^{93m}Mo isomer via the excitation of a 4.8 keV transition to an above lying triggering level that then decays via a fast cascade to the ground state.

As excitation mechanisms we consider the competition between photoexcitation and the coupling to the atomic shell in the process of nuclear excitation by electron capture (NEEC). A brilliant x-ray free electron laser (XFEL) source delivers the resonant photons for photoexcitation and simultaneously produces the electron plasma [1] which provides the free electrons and charged ions necessary for NEEC. Based on the semi–classical Maxwell–Bloch equations and perturbation theory we present numerical results for reaction rates of isomer depletion. While the photoexcitation cross section is typically two orders of magnitude smaller than the NEEC one for the 4.8 keV transition [2], we show that the efficiency of the NEEC process is in our case limited by the available charge states and the electron temperature in the plasma.

[1] S. M. Vinko *et al.*, Nature 482, 59 (2012).
[2] A. Pálffy, J. Evers and C. H. Keitel, Phys. Rev. Lett. 99, 172502 (2007).

A 30.6 Wed 16:00 Empore Lichthof

Conditions for orientation recovery using diffusion map — •Martin Winter, Ulf Saalmann, and Jan-Michael Rost — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Upcoming X-ray free electron lasers offer the potential of single-molecule coherent diffractive imaging without prior crystallization of the molecule. Since the molecules are in the gas phase, their orientations vary from shot to shot and the averaging of faint images from similar orientations requires a reliable orientation recovery of each image.

Here we show that such an orientation recovery using diffusion map [1] works only under certain conditions. We apply diffusion map to ensembles of unorientated diffraction patterns and to coordinates of points in three dimensional space and quantify when orientation recovery breaks down. For a better understanding we investigate the metric underlying the mappings from orientations to diffraction patterns and coordinates, respectively.

[1] Optics Express, Vol. 20, Issue 12, pp. 12799-12826 (2012)

A 30.7 Wed 16:00 Empore Lichthof

Nonlinear X-Ray Optics: A Numerical Study Based on the Maxwell-Schrödinger Equations — •Paolo Longo and Jörg Evers — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

The interaction of intense X-ray light (e.g., from a free-electron laser) with condensed matter does not only provide a versatile tool for the study of various material properties. It also allows for the investiga-

tion of coherent quantum optical effects in the X-ray domain [1]. In this work, we address questions from nonlinear X-ray optics based on a Maxwell-Schrödinger solver for quantum optical few-level systems [2].

[1] B. W. Adams *et al.*, J. Mod. Optic. *(in press)*.

[2] R. Fleischhaker and J. Evers, Comput. Phys. Commun. **182**, 739 (2011).

A 30.8 Wed 16:00 Empore Lichthof

XUV/IR pump-probe and single XUV photon dissociative ionization of H_2 — •Alexander Sperl[1], Andreas Fischer[1], Philipp Cörlin[1], Michael Schönwald[1], Arne Senftleben[1], Joachim Ullrich[1,2], and Robert Moshammer[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

Using a pump-probe scheme of an XUV-pump and IR-probe pulse, we investigated the nuclear wave packet dynamics of the high vibrational states in the $H_2^+(X\,^2\Sigma_g)$ potential. We observed the beating of the nuclear wave-packet as well as the de-phasing and re-phasing of the wave packet caused by the anharmonicity of the potential. By Fourier-transforming the time signal, we obtained the frequency spacings of the different vibrational states. We further studied the dissociative ionization induced by a single XUV photon. Here the doubly excited states Q_1 were mainly under investigation. In an ion-electron-correlation measurement we observed an oscillatory molecular frame asymmetry in the dissociation, similar to [1]. The asymmetry is caused by the interference of two paths.

Both measurements were performed using a reaction microscope, enabling the kinematically complete reconstruction of all momenta in a reaction.

[1] F. Martín, J. Fernández, T. Havermeier, L. Foucar, T. Weber, K. Kreidi, M. Schöffler, L. Schmidt, T. Jahnke, O. Jagutzki, et al., Science 315, 629 (2007)

A 30.9 Wed 16:00 Empore Lichthof

Towards Non-Linear X-ray Quantum Optics with Thin Film Cavities — •Kilian Heeg and Jörg Evers — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Thin film cavities with resonant iron-57 Mößbauer nuclei have proven to be a powerful system to study coherent light-matter interaction in the x-ray regime. Superradiance and the collective Lamb shift [1], electromagnetically induced transparency [2] and spontaneously generated coherences could be observed recently. In order to provide a full interpretation of the processes in the cavity, we establish a general quantum optical theory. This also opens the door to study quantum effects and the non-linear regime in such cavities. We discuss approaches and possible applications of this framework with the aim to determine if non-classical light states can be created in thin film cavities.

[1] R. Röhlsberger et al., Science 328, 1248-1251 (2010)
[2] R. Röhlsberger et al., Nature 482, 199 (2012)

A 30.10 Wed 16:00 Empore Lichthof

Dynamics of heteronuclear clusters in strong X-ray pulses — •Pierfrancesco Di Cintio, Ulf Saalmann, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We study the fragmentation dynamics of various molecular clusters (like CH_4, NH_3, H_2O) following multiple ionization with short and intense X-ray pulses. Whereas the photons are preferentially absorbed by the core electrons of the heavy species in the cluster, fast intramolecular charge transfer results in the formation of bare protons. We observe low final charge states of the heavy atoms and an intensity-dependent segregation of the proton and heavy-atom component leading to an inhibited expansion of the latter. Such findings could be relevant to approach the damage processes of large organic molecules as they occur during coherent diffractive imaging with intense X-ray pulses.

A 30.11 Wed 16:00 Empore Lichthof

Circular polarimetry of gamma-rays - a possible tool for observation of bulk antimatter in the Universe — •Stanislav Tashenov — Physics Institute, Heidelberg University, Germany

A significant body of observations points out that the Universe is composed of matter rather than antimatter. This baryon asymmetry for a long time remains an unsolved problem of physics. The current explanations include a possible CP-symmetry violation or a perfect separation between the bulks of matter and antimatter in the Universe. In the latter case this separation would preclude an observation of annihilation radiation at the border regions. This radiation is currently the only probe for bulk antimatter and it may fail if no bulk matter is present in the vicinity. Another possible method which is free from this limitation is based on circular polarimetry of gamma-rays, in particular on the circular polarization of gamma-ray continuum afterglow which follows a supernova explosion. However, so far no technique to measure circular polarization of cosmic gamma-rays was available. I propose the first such technique which can be naturally integrated into the concept of a gamma-ray Compton telescope. It is based on the transfer of the gamma-ray spin to the recoiled electron in Compton scattering and subsequent detection of the electron spin polarization by means of bremsstrahlung of these electrons. The physics phenomena needed by this technique were recently confirmed and the necessary algorithm for polarization reconstruction was developed.

A 30.12 Wed 16:00 Empore Lichthof

A high precision experimental benchmark of Fe M-shell unresolved-transition-array (UTA) inter-shell absorption lines — C. Beilmann[1], M. Leutenegger[2], R. Steinbrügge[1], J. Rudolph[1,3], S. Eberle[1], M.C. Simon[1], S.W. Epp[1], A. Graf[4], G.V. Brown[4], P. Beiersdorfer[4], T.M. Baumann[1], F.R. Brunner[1], S. Bernitt[1], Z. Harman[1,5], N.S. Oreshkina[1], C.H. Keitel[1], R. Follath[6], G. Reichardt[6], J. Ullrich[1], and •J.R. Crespo López-Urrutia[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]NASA/GSFC, Greenbelt MD, USA — [3]Universität Gießen, Germany — [4]LLNL, Livermore CA, USA — [5]EMMI, Darmnstadt, Germany — [6]HZB/BESSY, Berlin, Germany

Measurements of inner-shell absorption lines in highly charged ions have been performed with the portable electron beam ion trap FLASH-EBIT. It was coupled to a high-resolution monochromator at the synchrotron X-ray source BESSY II [1] to measure the resonant excitation energies of states decaying by autoionization or photon emission, which are measured by counting photoions and fluorescence photons in dependence of the X-ray energy. We compared the results with those of our own state-of-the-art relativistic configuration-interaction and multiconfiguration Dirac-Fock calculations, as well as with other recent calculations. The experimentally determined resonance energies typically have absolute precisions of about 70 meV, stringently benchmarking theory.

[1] M.C. Simon et al., Phys. Rev. Lett. **105**, 183001 (2010)

A 30.13 Wed 16:00 Empore Lichthof

X-ray spectroscopy of chemical systems in liquids phase — •Zhong Yin[1,2], Simone Techert[1], Ivan Rajkovic[1], Katharina Kubicek[1,2], Alexander Föhlisch[3,4], Philippe Wernet[3], and Wilson Quevedo[3] — [1]Max Planck Institute for Biophysical Chemistry, Am Faßberg 11, 37077 Göttingen, Germany — [2]Deutsches-Elektron Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]Helmholtz Zentrum Berlin, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [4]University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam, Germany

Based on their ability to salt in or salt out macromolecules salt ions are classified according to the Hofmeister series. While the macroscopic effect is known for over 100 years, the origin of the effect on the molecular level is still not understood. We present X-ray emission spectroscopy (XES) on the oxygen K-edge of water in aqueous solutions of inorganic salts using BESSY II synchrotron (Berlin, Germany) X-rays. The FlexRIXS end station utilized a liquid micro jet for sample delivery. The element- and site-specific XES method contains information about occupied and unoccupied molecular orbitals and is therefore sensitive to the chemical environment. The aim of our measurements was to reveal the influence of the water-ion interactions on the local water structure further elucidating the understanding of the structure maker and structure breaker concept. Structural changes while utilizing different salts were expected to show as spectral changes in the oxygen K-edge spectra, e.g. of peak shapes or intensities.