A 24: Poster: Interaction with VUV and X-ray light

Time: Wednesday 16:30–19:00 Location: Poster.V

A 24.1 Wed 16:30 Poster.V

Relativistic calculations of atomic transition, ionization and recombination properties — •Stephan Fritzsche — GSI Helmholtzzentrum für Schwerionenforschung & Frankfurt Institute for Advanced Studies, Germany; Department of Physics, University of Oulu, Finland

The Ratip program has been developed during the past years to calculate the electronic structure and properties of atoms and ions [1]. Today, this program provides a powerful platform in order to generate and evaluate atomic data for open-shell atoms, including level energies and energy shifts, transition probabilities, Auger parameters as well as a variety of excitation, ionization and recombination amplitudes and cross sections. Although the Ratip program focus on properties with just *one* electron within the continuum, recent emphasis was placed also on second-order processes as well as those properties for which different types of (many-electron) amplitudes need to be combined in order explain complex spectra at synchrotron and FEL light sources. Here, I present and discuss the (design of the) Ratip program, of which a major part now becomes public. Selected examples refer to the — direct and sequential — double ionization of various atoms [2,3].

[1] S. Fritzsche, submitted to Comput. Phys. Commun. (2011).
[2] P. Linusson et al., Phys. Rev. A **83** (2011) 023424.
[3] S. Fritzsche et al., J. Phys. B **44** (2011) 175602.

A 24.2 Wed 16:30 Poster.V

Two-photon absorption of few-electron heavy ions — Andrey Surzhykov[1,2], Paul Indelicato[3], Jose-Paulo Santos[4], Pedro Amaro[4], and •Stephan Fritzsche[2,5] — [1]Physikalisches Institut, Universität Heidelberg, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung, Germany — [3]Laboratoire Kastler Brossel, Paris, France — [4]Departamento de Física, Universidade Nova de Lisboa, Portugal — [5]Department of Physics, University of Oulu, Finland

The two-photon absorption of few-electron ions has been studied theoretically in the framework of second-order perturbation theory and Dirac's relativistic equation. Expressions were derived especially for the excitation cross sections and rates, including the contribution of higher-order multipoles in the expansion of the electron-photon interaction. Though these expressions are independent of the particular shell structure of the ion, detailed computations have been carried out for the two-photon absorption of hydrogen-, helium-, and berylliumlike ions and are compared with the available theoretical and experimental data. In this contribution, we discuss the relativistic and nondipole effects upon the induced two-photon transitions as well as the potential for exploring parity-violating interactions in high-Z ions [1].

[1] A. Surzhykov et al., Phys. Rev. A **84** (2011) 022511.

A 24.3 Wed 16:30 Poster.V

Photon-ion spectrometer PIPE at the Variable Polarization XUV Beamline of PETRA III — •Stefan Schippers[1], Sándor Ricz[1,2], Ticia Buhr[1,3], Jonas Hellhund[1], Alfred Müller[1], Stephan Klumpp[4], Karolin Mertens[4], Michael Martins[4], Roman Flesch[5], Eckart Rühl[5], Julian Lower[6], Till Jahnke[6], Daniel Metz[6], Lothar Ph. H. Schmidt[6], Reinhard Dörner[6], Alexander Dorn[7], and Andreas Wolf[7] — [1]Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Gießen — [2]ATOMKI, Debrecen, Hungary — [3]PTB, Braunschweig — [4]Institut für Experimentalphysik, Universität Hamburg — [5]Institut für Chemie und Biochemie, Freie Universität Berlin — [6]Institut für Kernphysik, Johann-Wolfgang-Goethe Universitä Frankfurt — [7]Max-Planck-Institut für Kernphysik, Heidelberg

The Photon-Ion spectrometer at PETRA III (PIPE) is a newly built permanent end station at the Variable Polarization XUV Beamline (P04) of the third-generation synchrotron light source PETRA III in Hamburg. Mass/charge selected atomic, (bio)molecular and cluster ions with masses of up to 30000 u, and neutral species can be used as targets for the study of the interaction of gaseous matter with linearly and circularly polarized photons in the energy range 250–3000 eV. State-of-the-art photo-product detection techniques are employed, such as COLTRIMS, high-resolution electron spectroscopy, and fluorescence detection. Details will be presented on the poster.

A 24.4 Wed 16:30 Poster.V

Traptor - A Multipole Radiofrequency Trap for PIPE, the ion beam facility at PETRA III — Alexander Guda[1,2], •Ricarda Laasch[1], Stephan Klumpp[1], and Michael Martins[1] — [1]Universität Hamburg, Institut für Experimentalphysik, Hamburg — [2]Southern Federal University, Rostov-on-Don, Russia

The ion beam facility PIPE (Photo-Ion-Spectrometer at PETRA III) at the P04 beamline of the synchrotron storage ring PETRA III, DESY, Hamburg, is able to prepare mass selected ion beams up to particles with 30.000amu of weight with an mass resolution up to 500 for x-ray absorption studies.
Usually, the more complex and heavy the ion of choice becomes, the more diluted is the prepared ion beam, making it harder or impossible to detect an absorption or fragmentation signal. A possible solution is to catch the ions of the prepared beam in an ion trap over a distinct time to enhance the density of particles for the interaction increasing the signal-to-noise ration significantly [1].
We build an 16-pole segmented radio-frequency ion trap (Traptor) [2] for PIPE. We will show using simulations with SimIon that the presented concept of Traptor is capable of trapping the range of masses PIPE can prepare as well as eject produced fragments in the trap after excitation with synchrotron radiation efficiently with a gradient field applied at the different segments. First tests of the setup in the laboratory will be presented.

[1] D. Gerlich, Advances in Chemical Physics, 82:1-176 (1992)
[2] K. Hirsch et. al., J. Phys. B., 42(15), 154029 (2009)

A 24.5 Wed 16:30 Poster.V

Fragmentation dynamics of molecular ions containing inner-shell ionized sulphur — •Arne Senftleben[1], Kirsten Schnorr[1], Moritz Kurka[1], Georg Schmid[1], Benjamin Erk[2], Artem Rudenko[2], Tatiana Marchenko[3], Marc Simon[3], Claus-Dieter Schröter[1], Robert Moshammer[1], and Joachim Ullrich[1] — [1]Max-Planck-Institut f. Kernphysik, Heidelberg — [2]Max-Planck Advanced Study Group, Hamburg — [3]LCPMR, Paris

The sulphur-containing molecules OCS and SF_6 have been ionized by intense radiation of 200 eV photons from the free-electron laser in Hamburg (FLASH). The photon energy is sufficient to eject a sulphur 2p electron, leading to auto-ionization of one or more other electrons and consequently to dissociation of the molecule. Using a reaction microscope, we have measured photo-electrons in coincidence with the ionic fragments. This enables us to study interrelations between electron spectra and the fragmentation channel of the remaining ion. For OCS, molecular-frame photo-electron angular distributions can be shown, while in SF_6 traces of non-linear processes will be discussed.

A 24.6 Wed 16:30 Poster.V

Time-dependent theory of strong-field x-ray resonance fluorescence — •Stefano M. Cavaletto[1], Christian Buth[2], Zoltán Harman[1,3], and Christoph H. Keitel[1] — [1]Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany — [2]Argonne National Laboratory, Argonne, Illinois 60439, USA — [3]ExtreMe Matter Institute EMMI, Planckstrasse 1, D-64291 Darmstadt, Germany

Resonance fluorescence is the emission of photons scattered off by atoms and molecules driven by a near-resonant external electric field; it is a cornerstone of x-ray spectroscopy and x-ray quantum optics. For intense x rays like those provided by existing and upcoming XFELs, the stimulated excitation and recombination at the Rabi frequency can compete with radiative and Auger decay. The signature of Rabi flopping in the electron spectrum of resonant Auger decay was studied for a two-level model of neon cations driven strongly by LCLS light tuned to the $1s\,2p^{-1} \rightarrow 1s^{-1}\,2p$ transition at 848 eV [1, 2]. Because of the advantages of photon detection over electron detection, we perform a time-dependent study of the spectrum of resonance fluorescence for neon cations, by considering two different scenarios, i.e. the chaotic pulses presently generated at LCLS and the coherent pulses which are going to become available in the near future via seeding techniques.

[1] N. Rohringer and R. Santra, Phys. Rev. A **77**, 053404 (2008).
[2] E. P. Kanter *et al.*, Phys. Rev. Lett. **107**, 233001 (2011).

A 24.7 Wed 16:30 Poster.V

Theory of field-assisted post-collision interaction in Auger

decay of atoms — •Sebastian Bauch[1], Bernd Schütte[2,3], Ulrike Frühling[2], Markus Drescher[2], and Michael Bonitz[1] — [1]Christian-Albrechts-Universität Kiel — [2]Universität Hamburg — [3]Max-Born-Institut Berlin

Post-collision interaction (pci) is a three-body effect being present in photo-induced Auger decay if the Auger electron (AE) is significantly faster than the preceding photoelectron (PE). Under these conditions, the AE experiences a rapid change of the ion's potential upon overtaking of the PE due to altered screening. This is connected with an exchange of energy between both electrons, the net amount of which depends on the AE's release time.

Utilizing extensive simulations based on the time-dependent Schrödinger equation as well as classical molecular dynamics, we show that pci, in the presence of a laser field, imprints a non-linear negative chirp on the AE's energy. Our theoretical results are in good agreement with recent experiments based on the light-driven THz streak camera [1,2] for MNN decay in Krypton and NOO decay in Xenon. The physical mechanism is explained within an analytical model for the line shape of the Auger electron, incorporating the effect of field-assisted pci.

[1] U. Frühling et al., Nat. Photon. 3 523 (2009)

[2] B. Schütte et al., submitted to Phys. Rev. Lett. (2011)

A 24.8 Wed 16:30 Poster.V

Ordering of randomly orientated diffraction patterns with diffusion map — •Martin Winter, Ulf Saalmann, and Jan-Michael Rost — Max-Planck-Institut für Physik komplexer Systeme, Dresden

By means of manifold embedding techniques we recover the orientations of an ensemble of diffraction patterns from a randomly orientated molecule, which would be the outcome of experiments at X-ray free-electron lasers. Since the mapping of the orientation to the diffraction pattern is highly non-linear, we use an algorithm capable of dealing with non-linear data, like diffusion map [1].

Diffusion map can handle a certain degree of non-linearity. Problems arise especially when multiple parameters/angles get mixed up in the mapping/formation of the diffraction patterns [2]. This is illustrated with some simple examples which reveal the applicability of diffusion map for scattering problems.

[1] Ronald R. Coifman, Stéphane Lafon, Diffusion maps, Appl. Comp. Harm. Anal. 21 (2006) 5-30

[2] Amit Singer, Ronald R. Coifman, Non-linear independent component analysis with diffusion maps, Appl. Comp. Harm. Anal. 25 (2008) 226-239

A 24.9 Wed 16:30 Poster.V

Cluster Sources for the Low Density Matter Beamline at the FERMI Free Electron Laser — •Raphael Katzy, Viktor Lyamayev, Marcel Mudrich, and Frank Stienkemeier — Universität Freiburg, Physikalisches Institut, D-79104 Freiburg, Germany

Applying high gain harmonic generation process (HGHG) the new FERMI free electron laser in Trieste provides intense XUV pulses of high brilliance with tunable wavelength and excellent confinement in time.

The LDM endstation has been designed to combine the FERMI XUV radiation with molecular beam experiments. In several exchangeable beam sources, atomic, molecular and cluster beams are generated and can be doped by the pick-up technique in oven cells or in a laser ablation unit. Detailed information about the interaction with the FEL light is gathered by combined VMI, TOF and X-ray imaging detectors.

Design and characterization of two sources are presented: A versatile high temperature high pressure pulsed source is utilized for generation of atomic, molecular and cluster beams of various materials in a gas expansion or applying the seeded beams technique. A pulsed cryogenic source gives the opportunity to use helium droplets with their unique cold, superfluid properties.

A 24.10 Wed 16:30 Poster.V

Time-resolved photofragmentation of molecular iodine at FLASH — •Kirsten Schnorr[1], Arne Senftleben[1], Thomas Pfeifer[1], Artem Rudenko[2], Georg Schmid[1], Kristina Meyer[1], Moritz Kurka[1], Yuhai Jiang[1], Stefan Düsterer[3], Joachim Ullrich[1], Claus Dieter Schröter[1], and Robert Moshammer[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg — [2]Max-Planck Advanced Study Group, Hamburg — [3]DESY, Hamburg

A pump-probe experiment on the ultrafast photofragmentation of molecular iodine using an ultra-short XUV pulse at ≈ 14 nm delivered by the free-electron-laser facility FLASH and a femtosecond IR laser pulse at ≈ 800 nm was performed.

In order to trace the molecular dynamics as a function of the internuclear distance, the delay between XUV- and IR-pulse is varied. With a preceding IR-pulse the I_2 molecule is dissociated and further ionized via the absorption of multiple XUV photons. We observe charge states up to I_2^{15+} due to FEL-created 4d core holes followed by Auger cascades.

All reaction channels resulting in charged fragments can be followed by recoil ion momentum spectroscopy using a reaction microscope.

A 24.11 Wed 16:30 Poster.V

Autoionization of D2 molecules using ultra-short XUV pulses — •Andreas Fischer, Alexander Sperl, Michael Schönwald, Helga Rietz, Philipp Cörlin, Arne Senftleben, Thomas Pfeifer, Robert Moshammer, and Joachim Ullrich — Max-Planck-Institut für Kernphysik, Heidelberg

Wave packet dynamics of molecules can be studied by combining an XUV pulse source and a Reaction Microscope. A Reaction Microscope allows for coincident measurements of ions and electrons. Further more it is capable of measuring the three dimensional momentum of each charged particle created in a reaction. We used this to study the autoionization of doubly-excited D2 molecules. The coupling with the dissociative photoionization channels leads to a symmetry breaking in the observed electron and ion angular distributions. Autoionizations occur on the same time scale as the molecular motion, therefore the nuclei can no longer be regarded stationary. In order to study these processes we probed the molecules with XUV pulse trains with photon energies of up to 32eV. We also modified the duration of the XUV pulse trains by changing the duration of the generating infrared pulses [1].

[1] J. Fernandez, F. Martin, New J Phys 11, 043020 (2009)

A 24.12 Wed 16:30 Poster.V

Gas-Based Photoemission Spectrometer for Online Shot-to-Shot Photon Beam Diagnostics at the European XFEL — •Jens Buck, Jan Grünert, Cigdem Ozkan, Bin Li, Wolfgang Freund, and Serguei Molodtsov — European XFEL GmbH, Albert-Einstein-Ring 19, 22761 Hamburg, Germany

At free-electron laser facilities, non-invasive beam diagnostics on the basis of photoionization of rare gases has found broad applications in the past and is also under development at the future European X-ray Free Electron Laser (XFEL.EU) facility [1,2]. The Self-Amplified Spontaneous Emission (SASE) process utilized here is known to produce pulses with significant statistical variations of essential pulse properties such as energy, spectrum, temporal profile etc. Single-pulse resolved diagnostics data is therefore required as an essential reference for user experiments. The specifications of XFEL.EU, especially the high intra-bunch repetition rate of 4.5 MHz and the vast energy range between 280 eV and 25 keV pose particular challenges for the design of gas-based devices.

We report on our conceptual design [3] and our recent developments of a photoelectron time-of-flight spectrometer for spectroscopy of single SASE pulses and give a first assessment of the expected performance of the device as derived from detailed simulations in a realistic environment and first commissioning experiments with synchrotron radiation.

[1] M. Altarelli et. al., *The European XFEL Technical Design Report* (2006). [2] J. Grünert, Proc. FEL09, Liverpool (2009). [3] J. Buck, *Conceptual Design Report: Photoemission Spectrometer*, in prep.

A 24.13 Wed 16:30 Poster.V

End-station for Low Density Matter Beamline at FERMI@Elettra Free Electron Laser — •Viktor Lyamayev, Raphael Katzy, Marcel Mudrich, and Frank Stienkemeier — Universität Freiburg, Physikalisches Institut, D-79104 Freiburg, Germany

FERMI@Elettra is a seeded type Free Electron Laser (FEL), which provides high brilliance femtosecond XUV-pulses in the 20-100 nm range with excellent temporal coherence and wavelength stability. Flexible tuning of both photon wavelength and polarization makes it unique tool for wide range of experiments.

The described setup will be installed as an end-station of the Low Density Matter beamline of FERMI@Elettra, which has been built for studying the interaction of FEL light with neutral molecular beams. It provides several types of sources for generating a wide range of atomic, molecular and cluster beams. Multiple pick-up cells as well

as laser ablation can be used for beam doping. A unique detection unit combines time-of-flight, velocity map imaging and X-ray imaging techniques. This allows simultaneous detection of electrons and ions as well as recording of X-ray diffraction patterns.

A 24.14 Wed 16:30 Poster.V

Few-photon multiple ionization of N_2 by 52 eV photons at FLASH — •Moritz Kurka[1], Artem Rudenko[2], Yuhai Jiang[1], Kai-Uwe Kühnel[1], Lutz Foucar[2], Arne Senftleben[1], Kirsten Schnorr[1], Georg Schmid[1], Oliver Herrwerth[3], Matthias Kling[3], Stefan Düsterer[4], Rolf Treusch[4], Claus Dieter Schröter[1], Robert Moshammer[1], and Joachim Ullrich[1,2] — [1]Max-Planck Institut für Kernphysik, 69117 Heidelberg — [2]Max-Planck Advanced Study Group at CFEL, 22607 Hamburg — [3]Max-Planck-Institut für Quantenoptik, 85748 Garching — [4]DESY, 22607 Hamburg

We report on the fragmentation of N_2 molecules induced by intense (10^{13}W/cm^2) XUV radiation ($\hbar\omega$ = 52eV) from the Free-Electron Laser in Hamburg (FLASH). Using a dedicated reaction microscope we detect the resulting ions and electrons in coincidence. The combined information contained in the energy and angular distributions of the emerging particles enables us to disentangle the various fragmentation pathways occurring. We will compare our results with those of Jiang et al. which were performed also at FLASH at a photon energy of 44 eV [1].

[1] Y.H. Jiang et *al., Phys. Rev. Lett.* ***102****, 123002 (2009).*

A 24.15 Wed 16:30 Poster.V

Interference of states with different symmetries and differently localized electrons in N_2O — •Andre Knie, Benjamin Kambs, Philipp Reiss, and Arno Ehresmann — Insitut für Physik und CINSaT der Universität Kassel, Heinrich-Plett-Str. 40 34132 Kassel, Germany

Quantum mechanical interference effects were investigated in N_2O, by photon-induced fluorescence spectroscopy. Energetically overlapping resonances of states with different symmetries and differently localized 1s core electrons of the center and terminal N atoms may interfere under certain conditions, breaking the symmetries by observing the processes in distinct angles in respect to the electric field of the exciting photon. Angularly and spectrally resolved fragment fluorescence spectra taken after inner shell excitation of overlapping resonances of core electrons of the central and terminal nitrogen atom indicate interference. In a second step the polarization of the fluorescence was measured to fortify the first measurements.

Results of the measurements are shown, as well as first interpretations of these interferences.