A 27: Poster: Photoionization

Time: Tuesday 16:30–18:30 Location: Spree-Palais

A 27.1 Tue 16:30 Spree-Palais

Radiative and Auger widths of X-ray K-shell excited few-electron iron ions — •René Steinbrügge[1], Sven Bernitt[1], Sascha W. Epp[2], Jan K. Rudolph[1,3], Christian Beilmann[5], Hendrik Bekker[1], Sita Eberle[1], Alfred Müller[3], Joachim Ullrich[6], Oscar O. Versolato[1], Hasan Yavaş[4], Hans-Christian Wille[4], and José R. Crespo López-Urrutia[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg — [3]Institut für Atom- und Molekülphysik, Gießen — [4]DESY, Hamburg — [5]Physikalisches Institut, Heidelberg — [6]PTB, Braunschweig

The spectrum of highly charged iron ions gives rich information of the dynamics of outflows in X-ray binary stars and active galactic nuclei. Very high X-ray fluxes in the vicinity of such objects produce and drive mainly photoionized plasmas, but up to now it was not possible to investigate the underlying photoionisation processes in the laboratory. We present the first measurement of radiative and Auger rates for K-shell transitions in Li-like, Be-like, and C-like iron ions. These were produced and trapped in the transportable electron beam ion trap FLASH-EBIT and resonantly excited with X-ray photons at PETRA III. We observe photoionization by detecting the changes in the ionic charge state. By taking ratios of the photoionization yield and the simultaneous recorded fluorescence, we suppress setup-dependent uncertainties. Together with the total linewidths [1], this allows us to determine absolute values for the radiative and Auger widths.

[1] J. K. Rudolph et al., Phys. Rev. Lett. **111**, 103002 (2013)

A 27.2 Tue 16:30 Spree-Palais

Präzisionsspektroskopie an der K-Kante astrophysikalisch relevanter Ionen — •Alfred Müller[1], Alexander Borovik[1], Kristof Holste[1], Jonas Hellhund[1], Dietrich Bernhardt[1], David Kilcoyne[2], Sandor Ricz[3], Stephan Klumpp[4], Michael Martins[4], Jens Viefhaus[5] und Stefan Schippers[1] — [1]Institut für Atom- und Molekülphysik, Universität Giessen — [2]Advanced Light Source, Berkeley, CA, USA — [3]ATOMKI Institute, Debrecen, Ungarn — [4]Institut für Experimentalphysik, Universität Hamburg — [5]FS-PE, DESY, Hamburg

Absolute Wirkungsquerschnitte für die Einfach- und Mehrfach-Ionisation von C^{q+} - Ionen mit q=1,2,3,4 und Ne^{q+}-Ionen mit q=1,2,3 durch einzelne Synchrotronstrahlungs-Photonen wurden an dem neu an PETRA III aufgebauten Photon - Ion Experiment PIPE (Photon - Ion Spectrometer at PETRA III) gemessen. Energieauflösungen der Photonenstrahlen bis herab zu 5 – 10 meV bei 330 eV wurden realisiert. Die abgedeckten Energiebereiche umfassen die niederenergetischsten mit Anregung eines K-Elektrons verknüpften Resonanzen bis hin zu autoionisierenden Zuständen mit Doppelanregung (K- und L-Schale) bei Energien jenseits der eigentlichen Ionisationskante der jeweiligen K-Schale. Emission von bis zu 3 Elektronen aus Ionen mit einem K-Loch wurde beobachtet. Im Fall von C^{4+} - Ionen wurden intermediäre Hohlatome (hohle Ionen) mit zwei Löchern in der K-Schale spektroskopiert.

A 27.3 Tue 16:30 Spree-Palais

PIPE - Absorption Spectroscopy of Small Molecular Ions — •Stephan Klumpp[1], Karolin Mertens[1], Michael Martins[1], Jonas Hellhund[2], Stefan Schippers[2], and Alfred Müller[2] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]Institut für Atom- und Molekülphysik, Universität Giessen

The Photon-Ion-Spectrometer at PETRA III (PIPE) at the XUV beamline P04, DESY, is a permanent end station dedicated to spectroscopic studies of free ions of various types, as atoms, molecular ions or mass selected clusters.

Using the merged-beams technique the prepared ion beam is collinear overlapped with x-ray photons from the P04 beamline between 250eV and 3000eV. This enables us to perform at PIPE absorption spectroscopy on the absolute scale in the region of the various inner shell absorption edges.

As a first case study for molecular ions the x-ray absorption and fragmentation of the IH^+ molecular ion at the Iodine 3d edge has been investigated. By comparing the IH^+ 3d partial cross section with the corresponding I^+ cross section strong deviations in the ion yield as well as in the shape of the partial cross section is found.

A 27.4 Tue 16:30 Spree-Palais

3d photoionization of ions from the Xe isonuclear sequence — •S Schippers[1], S. Ricz[2], T. Buhr[1,3], A. Borovik Jr.[1], J. Hellhund[1], K. Holste[1], D. Schury[1], S. Klumpp[4], K. Mertens[4], M. Martins[4], R. Flesch[5], G. Ulrich[5], E. Rühl[5], J. Lower[6], T. Jahnke[6], D. Metz[6], L. Ph. H. Schmidt[6], M. Schöffler[6], J. Williams[6], R. Dörner[6], L. Glaser[7], F. Scholz[7], J. Seltmann[7], J. Viefhaus[7], A. Dorn[8], A. Wolf[8], J. Ullrich[3] und A. Müller[1] — [1]IAMP, Univ. Giessen — [2]ATOMKI, Debrecen, Hungary — [3]PTB, Braunschweig — [4]Experimental Physics, Univ. Hamburg — [5]Physical Chemistry, FU Berlin — [6]Atomic Physics, Univ. Frankfurt a. M. — [7]FS-PE, DESY, Hamburg — [8]MPIK, Heidelberg

The photon-ion merged-beams technique has been employed at the new Photon-Ion spectrometer at PETRA III (PIPE) for measuring multiple photoionization of Xe^{q+} (q=1–5) ions. Total ionization cross sections have been obtained on an absolute scale for the dominant ionization reactions of the type $h\nu + Xe^{q+} \rightarrow Xe^{r+} + (q-r)e^-$ with product charge states $q+2 \leq r \leq q+5$. Prominent ionization features have been observed in the photon-energy range 650–800 eV, which are associated with excitation or ionization of an inner-shell $3d$ electron. The well-known collapse of the $4f$ wave function causes dramatic changes in the spectra when going from low to high q. Corresponding single-configuration Dirac-Fock calculations agree quantitatively with the experimental cross sections for non-resonant photoabsorption, but fail to reproduce all details of the measured ionization resonance structures.

A 27.5 Tue 16:30 Spree-Palais

Photoionization and photofragmentation of multiply charged $Lu_3N@C_{80}^{q+}$ ions — •Jonas Hellhund[1], Sándor Ricz[2], Alexander Borovik Jr.[1], Kristof Holste[1], Stephan Klumpp[3], Michael Martins[3], Stefan Schippers[1], and Alfred Müller[1] — [1]I.A.M.P, Univ. Giessen, Germany — [2]Atomki, Debrecen, Hungary — [3]Experimental Physics, Univ. Hamburg, Germany

Photoionization and photofragmentation of $Lu_3N@C_{80}^{q+}$ ($q = 1, 2, 3$) endohedral fullerene ions has been studied using the new Photon-Ion spectrometer at PETRA III (PIPE). Solid endohedral fullerene material was evaporated inside an ECR ion source. The generated ions were mass/charge selected and the ion beam was merged with the photon beam from PETRA III beamline P04. Product-ion yields normalized to ion current and photon flux, i.e., relative cross sections, were measured as a function of photon energy. The experimental photon-energy range was 270–1700 eV. This range comprises the energies for $1s$ ionization of carbon and nitrogen as well as for $3d$-ionization of lutetium.

The measured spectra exhibit clear signatures of carbon K-shell excitation, but no signs of excitation or ionization of encapsulated N or Lu producing vacancies in the $1s$ and $3d$ shells, respectively, have been observed. This is in contrast to recent findings for photofragmentation of $Xe@C_{60}^+$ [1] at energies of 60–150 eV. We speculate that the carbon cage and the encaged Lu_3N molecule completely disintegrate into relatively small fragments after absorption of one energetic photon.

[1] R. A. Phaneuf et al., Phys. Rev. A **88**, 053402 (2013).

A 27.6 Tue 16:30 Spree-Palais

Non-dipole effects in multiphoton ionization of hydrogen atom in short superintense laser fields — •Eric O. Jobunga[1,2] and Alejandro Saenz[1] — [1]AG Moderne Optik, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Department of Mathematics and Physics , Technical University of Mombasa, P. O. Box 90420-80100, Mombasa, Kenya

The development of novel light sources has enabled the realization of high-precision experiments investigating various non-linear processes in the dynamics of atomic, molecular, and ionic systems interacting with high intense laser pulses. At high intensities or short wavelengths, the analysis of these experiments would definitely require a reliable non-perturbative solution of the time-dependent Schrödinger or Dirac equation. These solutions should consider both the temporal and the spatial intensity variations of the laser pulse.We have solved the non-relativistic time dependent Schrödinger equation for a ground state hydrogen atom interacting with short intense spatially and temporally resolved laser fields corresponding to the multiphoton ATI regime for a monochromatic source with $\lambda = 800$ nm. We shall analyse the effects of the A^2 term and the corresponding orders of the multipolar

expansion of the transiton matrix.

A 27.7 Tue 16:30 Spree-Palais

Interaction effects on dynamical localization in driven helium — Felix Jörder, Klaus Zimmermann, •Alberto Rodriguez, and Andreas Buchleitner — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

Dynamical localization prevents driven atomic systems from fast fragmentation by hampering the excitation process. We present numerical simulations within a collinear model of microwave-driven helium Rydberg atoms and prove that dynamical localization survives the impact of electron-electron interaction, even for doubly excited states in the presence of fast autoionization. We conclude that the effect of electron-electron repulsion on localization can be described by an appropriate rescaling of the atomic level density and of the external field with the strength of the interaction [1].

[1] F. Jörder, K. Zimmermann, A. Rodriguez, and A. Buchleitner, arXiv:1311.5742

A 27.8 Tue 16:30 Spree-Palais

Dynamical Asymmetries of Electron Emission in CEP stable and two-color fields — •Martin Laux, Marcus Held, Yonghao Mi, Christian Ott, and Thomas Pfeifer — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

Photoelectron emission asymmetry in strong-field atomic photoionization plays a key role for the understanding of light-matter interaction in general. These asymmetries are caused by the spatial symmetry breaking within the laser pulse, as it happens e.g. in a few-cycle pulse with a fixed carrier-envelope phase (CEP). Another way to create an asymmetric laser field even for longer pulses is the superposition of a pulse with its second harmonic. Tuning the delay between the two colors or varying the CEP affects the asymmetry of photoelectron emission, but in qualitatively different fashions as confirmed by model calculations. A monolithic, robust, and phase-stable setup to create second harmonic light and allowing the continuous adjustment of the relative phase between the fundamental 800 nm and the frequency-doubled 400 nm pulses will be presented. Such dynamical two-color pulses are used for the study of dynamical asymmetry effects in photoionization of atoms and simple molecules with a reaction microscope.

A 27.9 Tue 16:30 Spree-Palais

The $1s^{-1}2s^{-1}, 2p^{-1}$ shake up satellites in Argon — •R. Püttner[1], T. Marchenko[2], R. Guillemin[2], R. K. Kushawaha[2], L. Journel[2], G. Goldsztejn[2], D. W. Lindle[4], M. N. Piancastelli[2,5], J.-P. Rueff[2,3], D. Ceolin[3], and M. Simon[2,3] — [1]Freie Universität Berlin, Germany — [2]CNRS and UPMC, UMR 7614, Paris , France — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]University of Nevada, Las Vegas, USA — [5]Uppsala University, Sweden

Using a new experimental setup for high-resolution HAXPES in the gas phase, which is mounted at the GALAXIES beamline of SOLEIL, we investigated the $1s^{-1}2s^{-1}, 2p^{-1}$ shake up structures of Argon, The spectrum of the $1s^{-1}2p^{-1}$ shake up satellites is dominated by the np (n=4 to 7) Rydberg series converging towards the ionization thresholds $^1P_1$ and $^3P_{2,1,0}$, which are determined with high accuracy. Below the $1s^{-1}2s^{-1}$ thresholds the spectrum is dominated by the broad $1s^{-1}2s^{-1}(^{1,3}S)4s$ Rydberg states which are split by approximately 16 eV. Moreover, a number of narrow lines are observed above the $1s^{-1}2p^{-1}(^{1,3}P)$ thresholds. Based on their linewidths and splittings these narrow lines are assigned to $1s^{-1}2p^{-1}(^{1,3}P)3p^{-1}n'l'n''l''$ final states populated via double shake processes. In addition, $1s^{-1}2p^{-1}$ the shake up satellites are also observed in molecules (S $1s^{-1}2p^{-1}$ in H_2S, Cl $1s^{-1}2p^{-1}$ in CH_3Cl and CCl_4) showing that this is a rather general effect. This observation opens the exciting new possibility to study single-site double core-hole (SS DCH) states in Si, P, S, and Cl containing molecules using conventional photoelectron spectroscopy at synchrotron radiation facilities.

A 27.10 Tue 16:30 Spree-Palais

Photoionization of the beryllium atom — •Sita Nagina Eberle[1], Oscar O. Versolato[1], Lisa Schmöger[1], Matthias Kohnen[2], Maria Schwarz[1], Piet O. Schmidt[2,3], Joachim Ullrich[1,2], and José R. Crespo López Urrutia[1] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Institut für Quantenoptik, Leibniz Universität Hannover, Hannover, Germany

A source of beryllium photoions was built in order to sympathetically cool highly charged ions in a cryogenic Paul trap with them. A suitable process for this purpose is the two-photon ionization of neutral beryllium atoms that is achieved by a resonant excitation of the $1s^2 2s^2\ ^1S_0 \rightarrow 1s^2 2s 2p\ ^1P_1$ transition at 235 nm of the atom followed by the non-resonant transfer of an electron to the continuum. The laser system used for the excitation and consecutive ionization of the atom is based on frequency doubling twice an amplified diode laser system at 940 nm. Ion and fluorescence spectral lines were measured and compared to simple models that describe the data quite well, at least qualitatively. Regarding the two-photon ionization cross sections, it should be noted that neither our simple estimates nor more sophisticated theoretical models reproduce the present experimental results. Most probably the assumptions underlying those calculations (e.g., weak coupling of the excited state to the continuum) are not realistic for our experimental settings. However, the setup fulfills the required specifications, including beryllium safety measures, and has been implemented in the main experiment CryPTEx.

A 27.11 Tue 16:30 Spree-Palais

Nonlinear photo-ionization dynamics using MCTHDF and Time-dependent RASCI — •Christopher Hinz[1], David Hochstuhl[2], and Michael Bonitz[1] — [1]ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel — [2]d-fine GmbH, Opernplatz 2, D-60313 Frankfurt

As of now, the exact simulation of correlated quantum systems is inherently limited by the exponential growth of the state space with the particle number, and the resulting computational complexity—established as curse of dimensionality. It is therefore necessary to use an adapted approximation to mitigate this barrier, such as by using an ansatz for the many-particle state of the system. To methodically understand the implications of such an ansatz, it is required to strictly quantify its structural properties and their impact on the treated observables. As a first benchmark, we compare the structural properties of atomic states during photo-ionization for the FCI, MCTDHF [1,3] and TD-RASCI [2,3] methods. Particularly, we try to identify the cause of some already known deficiencies of the MCTDHF ansatz [1]. In the end, the detailed insight into the structure of these systems will allow one to guide the development of more advanced approximations.

[1] D. Hochstuhl, and M. Bonitz, J. Chem. Phys **134**(8) (2011)
[2] D. Hochstuhl, and M. Bonitz, JPCS **427**, 012007 (2013)
[3] D. Hochstuhl, C. Hinz and M. Bonitz, EPJ ST in press

A 27.12 Tue 16:30 Spree-Palais

Ionization yield in the resonant C 1s electron excitation range of chiral terpene molecules — •Christian Ozga[1], Benjamin Kambs[1], Kari Jänkälä[2,3], Philipp Schmidt[1], Andreas Hans[1], Philipp Reiss[1], André Knie[1], and Arno Ehresmann[1] — [1]Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology, Universität Kassel, D-34132 Kassel, Germany — [2]Department of Physics, University of Oulu, P.O. Box 3000, 90014 Oulu, Finland — [3]Institute for Experimental Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Inner shell C 1s electrons were excited in different chiral terpene molecules by monochromatized synchrotron radiation with an energy close to the C 1s electron ionization threshold. Undispersed fluorescence excitation within the range between 280 nm and 680 nm and relative ionization yields have been measured. The ionization yield measurements were compared to time dependent density functional theory calculations, revealing the site specificity of the resonant inner shell excitations. This site specificity is discussed as a means for the excitation of individual stereocenters in the investigated chiral molecules.