



Editorial

Special Issue "Interaction of Ionizing Photons with Atomic and Molecular Ions"

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The interaction of ionizing photons with atoms or ions is a fundamental process in nature, with laboratory, atmospheric and astrophysical implications. Much of the matter in the universe is in the ionized state and so the results of theoretical and experimental investigations of photoionization of ions are key for the understanding of a wide range of phenomena.

Atomic ions provide an ideal testing ground for the study of the interaction of photons with a many-body system as ions are perfectly reproducible and the basic interparticle interactions are well known. Systematic studies along isoelectronic and/or isonuclear sequences provide flexibility in experimental and theoretical efforts. Photons in the vacuum ultraviolet, extreme ultraviolet and x-ray regimes can have sufficient energy to excite inner-shell electrons or more than one electron at a time. Hence the study of the photon-ion interactions provides considerable insight into how the complex many-body correlation aspects of the processes can be understood and quantified. Where molecular ions are concerned the experimental and theoretical challenges are even more daunting and it is only in recent years that substantial progress is being made.

The study of ionizing photon-ion interactions in the laboratory requires sources of short wavelength to provide the necessary high-energy photons. In the well-known book "From X-Rays to Quarks" by Emile Segré (Nobel Prize winner in 1959) he states on Page 275 "In the 1920s we used to joke that good physicists, once passed to their heavenly rewards, would find apparatus in paradise which, with a twist of some knobs, would give electromagnetic radiation of any desired frequency, intensity, polarization, and direction of propagation".

Developments in short wavelength sources over the last few decades, are coming ever closer to realizing such a "heaven on earth", as far as science at short wavelengths is concerned! For example, photon sources such as laser plasmas, high harmonic generation, synchrotrons and now short wavelength Free Electron Lasers (FELs), are currently available to allow the interaction of ionizing photons with matter to be studied on widely varying photon energy, spatial and time scales. The exploitation of the new source capabilities has required innovative detector solutions. To guide and understand experiments, a concomitant development in theoretical modeling of their complex many-body nature is required.

In the book "Interactions of Ionizing Photons with Atomic and Molecular Ions", based on the proceedings of a Special Issue [1], papers are included which show a variety of recent developments in theory and experiment.

The first of five theoretical papers, written by Gryzlova et al. [2], investigates the photoionization of krypton by intense femtosecond duration pulses, for photon energies (50–80 eV) which lie below the 3d excitation threshold. Sequential ionization processes and results on the time evolution of the 4s and 4p valence shells of Kr and its ions (Kr+,

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Kr²⁺ and Kr³⁺) are described together with the resulting photoelectron spectra. The theoretical approach based on R-matrix calculations uses rate equations with photoionization cross sections in different charge and multiplet states. The study is a precursor to calculations for higher photon energies where the 3d excitation channel is open and Auger decay makes the dynamics more complex.

Experiments with FELs are often multi-shot in character, where the target systems interact with FEL short wavelength pulses differing from each other in random ways, due to the fact that the individual pulses build up from SASE (Self-Amplified-Spontaneous-Emission) processes. Katravulapally and Nikolopoulos [3] treat the effects of the FEL fluctuations for the special case of the 2s2p Li⁺ autoionization lineshape. They employ a perturbative statistical description of the atomic dynamics to investigate the effects of parameters such as peak-intensity, coherence time and pulse duration on the lineshape and the ionization yield.

Hofbrucker et al. [4] note that two-photon ionization is one of the most fundamental nonlinear processes in which two photons are simultaneously absorbed and an electron is emitted. They treat the problem of non-resonant two-photon ionization in magnesium and examine the energy dependence of the resulting photoelectron angular distributions and in particular the angular distribution near the nonlinear Cooper minimum.

Preliminary insights into angle-dependent and angle-integrated spin-polarized photoelectron fluxes, from fullerene anions, are presented by Dolmatov [5]. The characteristics of the phenomenon are discussed within the framework of a simplified semi-empirical methodology where the C₆₀ cage is modeled by a spherical annular potential. The key result is that photodetachment of fullerene anions may produce highly spin-polarized photoelectrons.

The final theoretical paper, by Gorczyca et al. [6], uses the R-matrix methodology to address inner-shell photodetachment of the negatively charged Na- anion near the L-edge threshold. Significant structures are found in the cross section, which are compared to experimental results. Many-body correlation effects are seen to be crucial to the behaviour of the photodetachment cross section.

Several papers deal with experiments carried out at synchrotron facilities on beamlines equipped to examine photon-ion interactions.

Photoelectron spectroscopy of ions remains challenging due to the low density of ion beams but offers advantages over ion yield experiments through the provision of partial photoionization cross sections. Penent et al. [7] describe improvements by a factor of ~20 to an existing cylindrical mirror analyzer, obtained by replacing channeltrons by large micro-channel plate detectors in order to perform parallel detection of electrons. The improved performance is illustrated by electron spectra obtained for Si⁺ and Xe⁵⁺ ions at SOLEIL.

Dedicated ion-yield merged photon ion setups at synchrotron facilities such as the Photon Factory (Japan), Aarhus (Denmark), SOLEIL (France) and the ALS at Berkeley (USA) have all contributed to extensive photoionization results for a wide range of atomic ions. The most recent such development is the Photon-Ion Spectrometer (PIPE) at PETRA III in Hamburg, which is capable of very high-resolution investigations over the 250 eV to 3000 eV photon range. In their paper [8] Schippers and Müller show the flexibility and capabilities of PIPE by reviewing recent work on atomic ions of astrophysical interest. Examples include L-shell photoionization of Fe $^+$, Fe $^{2+}$ and Fe $^{3+}$ ions and single and multiple K-shell photoionization of C $^-$, C $^+$, Ne $^+$ and Si $^{2+}$.

Absolute cross sections for K-shell photoionization of N⁺ in the 398 to 450 eV photon energy range are reported by Mosnier et al. [9]. The results were obtained from ion yields at the MAIA (Multi-Analysis Ion Apparatus) merged photon-ion beam apparatus at the SOLEIL synchrotron facility. A narrow spectral bandpass of 65 meV was used in the 1s \rightarrow 2p region near 400 eV and extended Rydberg series were observed above 415 eV. The results were interpreted using Multi-Configuration-Dirac-Fock and R-matrix theoretical approaches.

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Using the same MAIA set-up at SOLEIL, N²⁺ fragments were measured following nitrogen K-shell excitation in the molecular ion NH⁺. Carniato et al. [10] show how the high sensitivity of MAIA combined with the high spectral resolution achievable at SOLEIL helped to resolve vibrational structures in the molecular ion. Assignment of the observed resonances was achieved by a detailed ab initio theoretical analysis, including vibrational dynamics, of the core-to-valence and core-to-Rydberg excitations.

The last three papers describe results obtained with laser-produced plasmas.

Scally et al. [11] report on the results of a systematic study of the emission between 10 and 18nm from plasmas produced with Sn, Pb and lead-tin alloys targets, under a variety of laser irradiation conditions and alloy concentrations. The ion stages contributing to the emission are identified through a collisional radiative model and atomic structure codes. Results obtained with Nd:YAG laser irradiation are compared to optically thinner CO₂ laser plasmas.

Lu et al. [12] report on the photoabsorption spectrum of Bi $^{+}$ in the wavelength regime between 37 and 60 nm, recorded by the dual laser plasma technique where separate laser plasmas provide the backlighting short wavelength continuum and the absorbing ions. 5d \rightarrow 6p transitions from the ground state of Bi $^{+}$ provide the strongest features while transitions from low-lying excited states make small contributions.

The final paper [13] by Wong et al. investigates the use of the Colombant and Tonon Collisional Radiative (CR) Model for the understanding of laser-produced plasmas. The CR model allows ion distributions for a given temperature and density to be calculated. Plots of the collisional ionization, radiative recombination and three-body recombination rate coefficients, ion distributions and peak fractional populations for various elements are included. The importance of dealing correctly with ionization bottlenecks is stressed.

The book overall provides insight into the variety of investigations into the interaction of short wavelength photons with atomic and molecular ions now possible. It is anticipated that investigations of the interaction of energetic photons with ionized matter will further deepen, with the advent of several new FEL facilities under development and which are expected to drive many new innovations and discoveries in the study of light-matter interactions in the short wavelength regime.

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References

1. Special Issue "Interaction of Ionizing Photons with Atomic and Molecular Ions". Available online: https://www.mdpi.com/journal/atoms/special issues/atom ions (accessed on 7 December 2021).

- 2. Gryzlova, E.V.; Kiselev, M.D.; Popova, M.M.; Zubekhin, A.A.; Sansone, G.; Grum-Grzhimailo, A.N. Multiple Sequential Ionization of Valence n = 4 Shell of Krypton by Intense Femtosecond XUV Pulses. *Atoms* **2020**, *8*, 80.
- 3. Katravulapally, T.; Nikolopoulos, L.A.A. Effects of the FEL Fluctuations on the 2s2p Li⁺ Auto-Ionization Lineshape. *Atoms* **2020**, *8*, 35.
- 4. Hofbrucker, J.; Eiri, L.; Volotka, A.V.; Fritzsche, S. Photoelectron Angular Distributions of Nonresonant Two-Photon Atomic Ionization Near Nonlinear Cooper Minima. *Atoms* **2020**, *8*, 54.
- 5. Dolmatov, V.K. Spin-Polarized Photoelectron Fluxes from Fullerene Anions. *Atoms* **2020**, *8*, 65.
- Gorczyca, T.W.; Zhou, H.-L.; Hibbert, A.; Hasoglu, M.F.; Manson, S.T. Inner-Shell Photodetachment of Na⁻ Using R-Matrix Methods. Atoms 2020, 8, 60.
- 7. Penent, F.; Cubaynes, D.; Lablanquie, P.; Palaudoux, J.; Guilbaud, S.; Moustier, O.; Guigand, J.; Bizau, J.-M. Modification of a Cylindrical Mirror Analyzer for High Efficiency Photoelectron Spectroscopy on Ion Beams. *Atoms* **2020**, *8*, 63.
- 8. Schippers, S.; Müller, A. Photoionization of Astrophysically Relevant Atomic Ions at PIPE. Atoms 2020, 8, 45.
- 9. Mosnier, J.-P.; Kennedy, E.T.; Bizau, J.-M.; Cubaynes, D.; Guilbaud, S.; Blancard, C.; McLaughlin, B.M. Photoionization Cross-Sections of Carbon-Like N⁺ Near the K-Edge (390–440 eV). *Atoms* **2021**, *9*, 27.

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10. Carniato, S.; Bizau, J.-M.; Cubaynes, D.; Kennedy, E.T.; Guilbaud, S.; Sokell, E.; McLaughlin, B.; Mosnier, J.-P. Vibrationally and Spin-Orbit-Resolved Inner-Shell X-ray Absorption Spectroscopy of the NH⁺ Molecular Ion: Measurements and ab Initio Calculations. *Atoms* **2020**, *8*, 67.

- 11. Scally, E.; O'Reilly, F.; Hayden, P.; Tobin, I.; O'Sullivan, G. An Investigation of Laser Produced Lead-Tin Alloy Plasmas between 10 and 18 nm. *Atoms* **2020**, *8*, 75.
- 12. Lu, H.; Varvarezos, L.; Hayden, P.; Kennedy, E.T.; Mosnier, J.-P.; Costello, J.T. The 5d-6p VUV Photoabsorption Spectrum of Bi⁺. *Atoms* **2020**, *8*, 55.
- 13. Wong, N.L.; O'Reilly, F.; Sokell, E. Investigation of a Collisional Radiative Model for Laser-Produced Plasmas. *Atoms* **2020**, *8*, 52.