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Multi-electron processes in K-shell double and triple photodetachment of oxygen anions

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Synopsis Absolute cross sections for double and triple photodetachment of O^- ions have been measured at photon energies around the threshold for *K*-shell ionization using the photon-ion merged-beams technique at a synchrotron light-source. In addition, corresponding large-scale *ab-initio* calculations were carried out at a level of complexity that has never been invoked before. From the comparison between experiment and theory it becomes apparent that the inclusion of multi-electron processes such as double shake-up in the theoretical calculations is crucial for the explanation of the experimental findings.

Absolute cross sections of double and triple photodetachment of O^- ions were measured in the experimental photon energy range of 524–543 eV that comprised the threshold for K-shell ionization [1]. For the experimental measurements, the photon-ion merged-beams technique [2] was employed using the permanently installed end station PIPE [3] at the "Variable Polarization XUV Beamline" (P04) [4] of the synchrotron light source PETRA III at DESY in Hamburg, Germany. Using resolving powers of up to 13000, the position, strength and width of the below-threshold $1s\,2s^2\,2p^6\;{}^2S$ resonance (Fig. 1) as well as the positions of the $1s\,2s^2\,2p^5\;{}^3P$ and $1s\,2s^2\,2p^5\;{}^1P$ thresholds for K-shell ionization were determined with high-precision. In addition, systematically enlarged multi-configuration Dirac-Fock calculations have been performed for the resonant detachment cross sections by utilizing the MCDF method as implemented in the GRASP [5] and RATIP [6] codes. Results from these *ab initio* computations agree very well with the measurements for the resonance width and branching fractions for double and triple detachment, if *double* shake-up (and -down) of valence electrons and the rearrangement of the electron density is taken into account. For the absolute cross sections, however, a previously found discrepancy between measurements and theory is confirmed [1].

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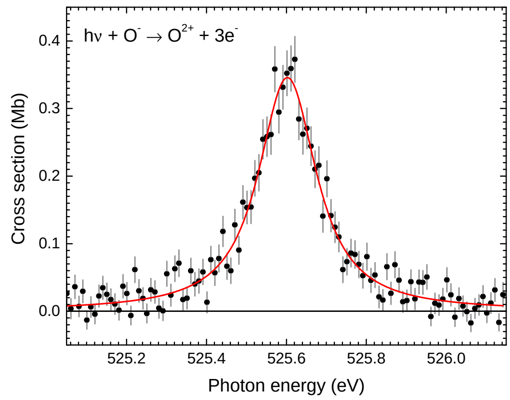

Figure 1. High-resolution measurement (symbols) of the $1s\,2s^2\,2p^6\;{}^2S$ resonance in the triple detachment channel [1]. The resonance width has been determined from a Voigt line-profile fit (line) to be 164 ± 14 meV.

References

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