

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

S. Schippers^{*†}, R. Beerwerth^{‡,‡}, L. Abrok[§], S. Bari^{‡,‡}, M. Martins[△],
S. Ricz[§], J. Viehhaus[‡], S. Fritzsche^{‡,‡}, A. Müller[◇]

^{*} I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

[†] Helmholtz-Institut Jena, 07743 Jena, Germany

[‡] Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

[§] Institute of Nuclear Research of the Hungarian Academy of Sciences, 4026 Debrecen, Hungary

[‡] European XFEL GmbH, 22869 Schenefeld, Germany

[‡] DESY Photon Science, FS-SCS, 22607 Hamburg, Germany

[‡] DESY Photon Science, FS-PE, 22607 Hamburg, Germany

[△] Institut für Experimentalphysik, Universität Hamburg, 22761 Hamburg, Germany

[◇] Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

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 $1s2s^22p^6\ ^2S$ resonance (Fig. 1) as well as the positions of the $1s2s^22p^5\ ^3P$ and $1s2s^22p^5\ ^1P$ 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].

This research was carried out at the light source PETRA III at DESY, a member of the Helmholtz Association (HGF). We would like to thank G. Hartmann, F. Scholz, and J. Seltmann for assistance in using beamline P04 as well as S. Klumpp for his continuous support of the PIPE setup. Fund-

ing by BMBF (contracts 05K10RG1, 05K10GUB, 05K16RG1, 05K16GUC, and 05K16SJA) is gratefully acknowledged.

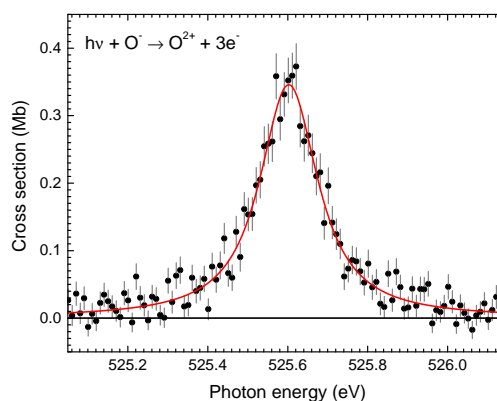


Figure 1. High-resolution measurement (symbols) of the $1s2s^22p^6\ ^2S$ resonance in the triple detachment channel [1]. The resonance width has been determined from a Voigt line-profile fit (line) to be 164 ± 14 meV.

References

- [1] S. Schippers *et al.* 2016 *Phys. Rev. A* **94** 041401(R)
- [2] S. Schippers *et al.* 2016 *Contemp. Phys.* **57** 215
- [3] S. Schippers *et al.* 2014 *J. Phys. B* **47** 115602
- [4] J. Viehhaus *et al.* 2013 *Nucl. Instrum. Meth. A* **710** 151
- [5] P. Jönsson *et al.* 2007 *Comput. Phys. Commun.* **177** 597
- [6] S. Fritzsche 2012 *Comput. Phys. Commun.* **183** 1525

[†]E-mail: stefan.schippers@physik.uni-giessen.de

