The all-seeing eye of Auger electron spectroscopy: a study on aqueous KCl

Tsveta Miteva,[†] Nikolai Kryzhevoi,[‡] Nicolas Sisourat,[†] Christophe Nicolas,[¶] Wandared Pokapanich,[§] Th. Saisopa,[‖] P. Songsiriritthigul,[‖] Y. Rattanachai,[⊥] Andreas Dreuw,[#] Jan Wenzel,[#] Jérôme Palaudoux,[†] Gunnar Öhrwall,[†] Ralph Püttner,[@] Lorenz S. Cederbaum,[‡] Jean Pascal Rueff,[†] and Denis Céolin*[,¶]

†*Sorbonne Universités, UPMC Univ Paris 06, UMR 7614, Laboratoire de Chimie Physique Matière et Rayonnement, F-75005 Paris, France*

‡*Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany*

¶*Synchrotron SOLEIL, l'Orme des Merisiers, Saint-Aubin, F-91192 Gif-sur-Yvette Cedex, France*

§*Faculty of Science, Nakhon Phanom University, Nakhon Phanom 48000 Thailand*

‖*NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials and School of Physics, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand*

⊥*Department of Applied Physics, Faculty of Sciences and Liberal Arts, Rajamangala University of Technology Isan, Nakhon Ratchasima 30000, Thailand*

#*Interdisciplinary Center for Scientific Computing, Ruprecht-Karls University, Im Neuenheimer Feld 205A, D-69120 Heidelberg, Germany*

@*Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195, Berlin, Germany*

E-mail: denis.ceolin@synchrotron-soleil.fr

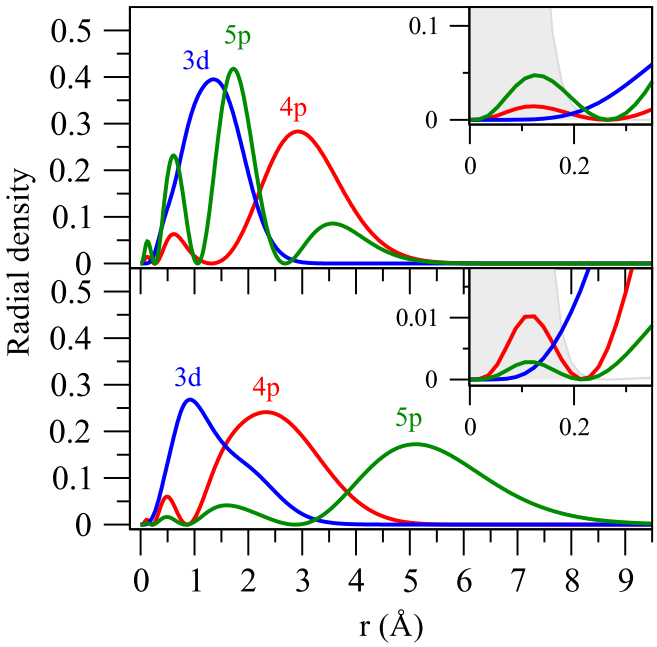

Figure 1: Radial density distributions of the singly-occupied natural orbital occupied by the excited electron corresponding to the 1s→4p, 1s→3d and 1s→5p core excitations in K^+ (lower panel) and Cl^- (upper panel). The insets show the region of distances relevant for the overlap with the 1s core orbital whose radial density is shown as a grey shaded area.

References

(1) Föhlisch, A.; Feulner, P.; Hennies, F.; Fink, A.; Menzel, D.; Sanchez-Portal, D.; Echenique, P. M.; Wurth, W. *Nature 436*, 373.

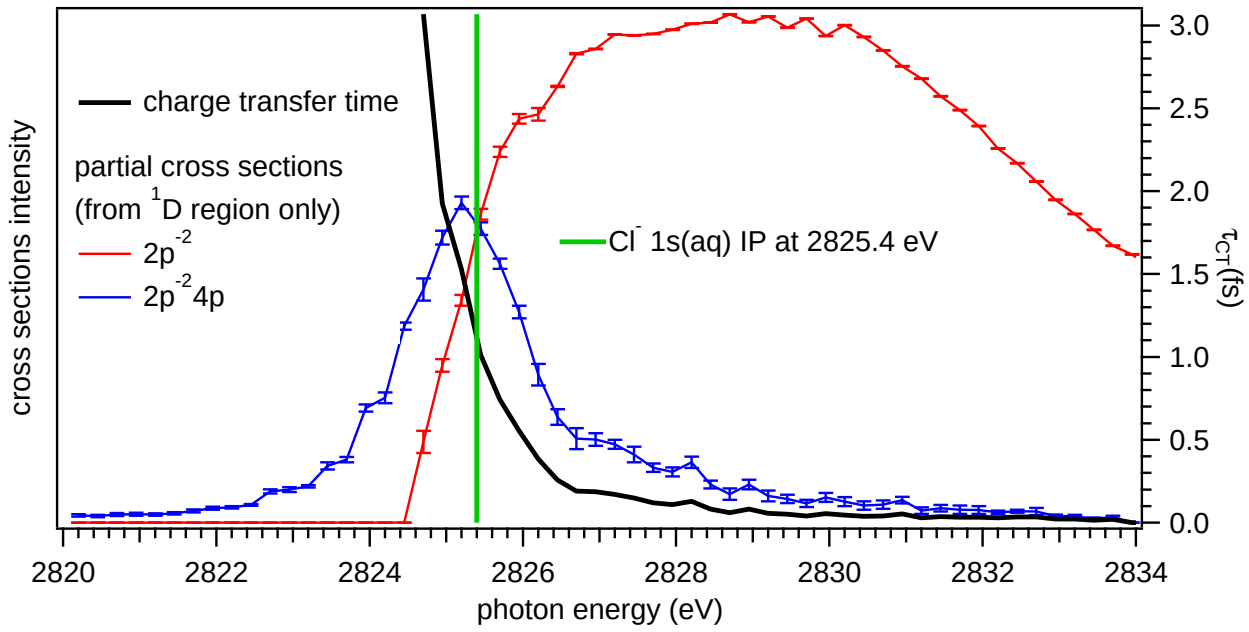

Figure 2: Partial cross sections and charge transfer time extracted from Fig. **??**. The blue and red curves are obtained by integrating the area of the $2p^{-2}$ and $2p^{-2}4p$ final states (^1D state region only) at each photon energy step. From these curves we determine the charge transfer time τ_{CT} according to the formula $\tau_{CT} = \tau l/d$, with τ being the Cl 1s core-hole lifetime and l/d being the intensity ratio of the localized ($2p^{-2}$ 4p) and delocalized ($2p^{-2}$) states at a given excitation energy.[1] The green line defines the $Cl^-_{aq}(1s)$ ionization potential.