The all-seeing eye of resonant 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 Université, CNRS, Laboratoire de Chimie Physique Matière et Rayonnement, UMR 7614, F-75005 Paris, France

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

 $\P Synchrotron\ SOLEIL,\ l'Orme\ des\ Merisiers,\ Saint-Aubin,\ F-91192\ Gif-sur-Yvette\ Cedex,$ 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

\(\perp \)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

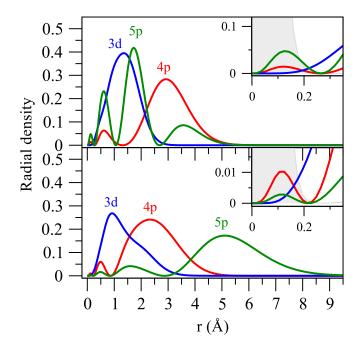


Figure 1: Radial density distributions of the singly-occupied natural orbital occupied by the excited electron corresponding to the $1s\rightarrow 4p$, $1s\rightarrow 3d$ and $1s\rightarrow 5p$ core excitations in K^+ (lower panel) and Cl^- (upper panel). The insets show the region of distances relevant 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.

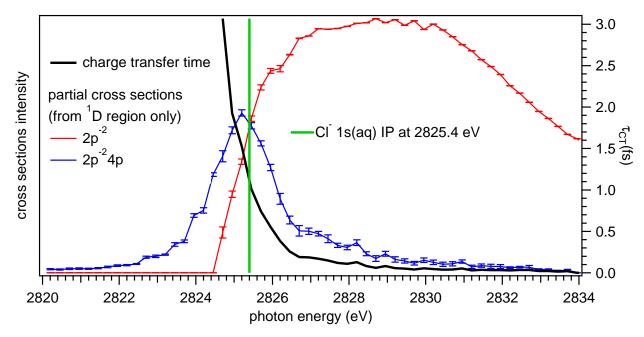


Figure 2: Partial cross sections and charge transfer time extracted from Fig. ??. The blue and red curves are obtained by integrating the area of the $2p^{-2}$ and $2p^{-2}4p$ final states (¹D state region only) at each photon energy step. From these curves we determine the charge transfer time $\tau_{\texttt{CT}}$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