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

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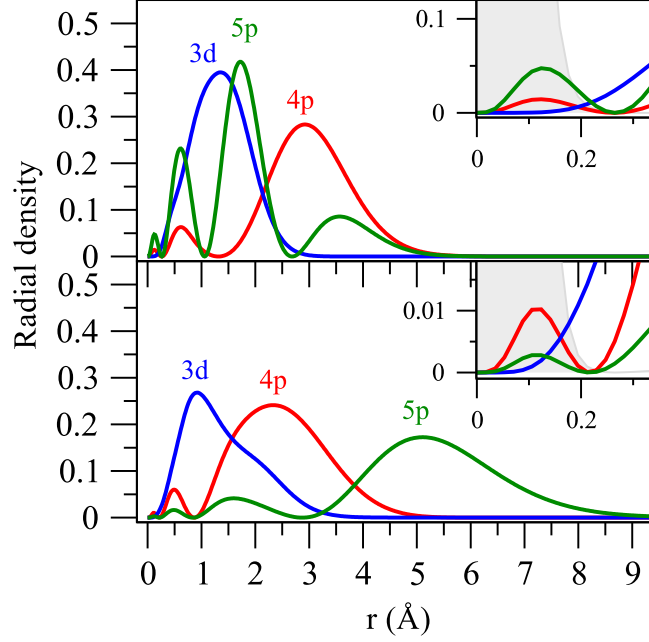E-mail: tsveta.miteva@upmc.fr; denis.ceolin@synchrotron-soleil.fr

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.
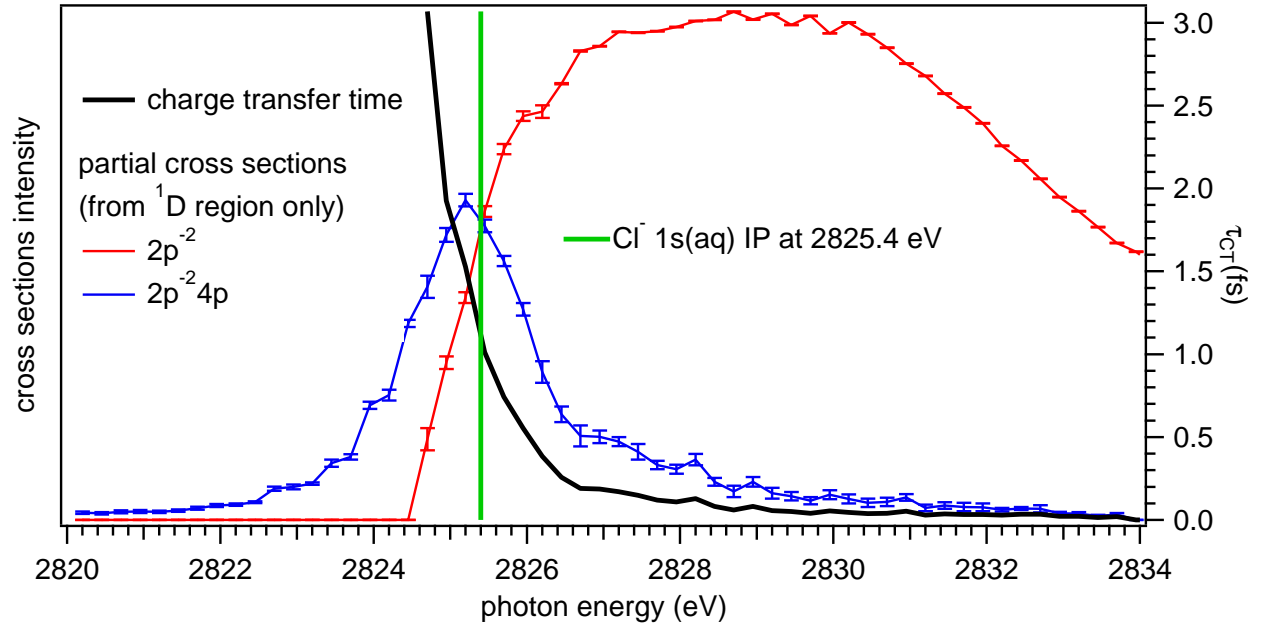
Figure 2: Partial cross sections and charge transfer time extracted from Fig. **??**. The blue and red curves are obtained by integrating the area of the $2p^{-2}$ and $2p^{-2}4p$ final states (^{1}D state region only) at each photon energy step. From these curves we determine the charge transfer time τ_{CT} according to the formula $\tau_{\mathrm{CT}} = \tau l/d$, 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 $\mathrm{Cl}^-_{\mathrm{aq}}$(1s) ionization potential.