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

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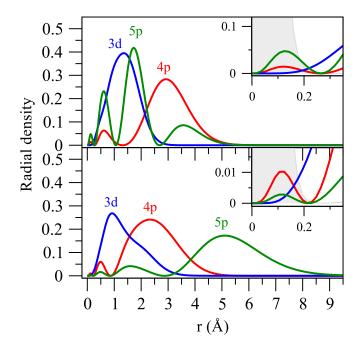


Figure 1: Radial density distributions of the singly-occupied natural orbital occupied by the excited electron corresponding to the $1s\rightarrow 4p$, $1s\rightarrow 3d$ and $1s\rightarrow 5p$ core excitations in K^+ (lower panel) and Cl^- (upper panel). The insets show the region of distances relevant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

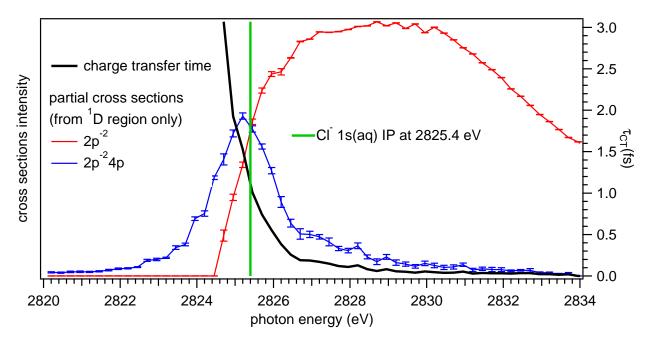


Figure 2: Partial cross sections and charge transfer time extracted from Fig. ??. The blue and red curves are obtained by integrating the area of the $2p^{-2}$ and $2p^{-2}4p$ final states (^{1}D state region only) at each photon energy step. From these curves we determine the charge transfer time $\tau_{\rm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