The electronic structure of aqueous KCl revealed by X-ray absorption and Auger electron spectroscopy

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

Tsveta Miteva,[†] Nikolai Kryzhevoi,[‡] Nicolas Sisourat,[†] Ch. Nicolas,[†] Wandared Pokapanich,[†] Th. Saisopa,[†] P. Songsiriritthigul,[†] Y. Rattanachai,[†] Andreas Dreuw,[¶] Jan Wenzel,[¶] Ralph Püttner,[†] Jérôme Palaudoux,[†] Gunnar Öhrwall,[†] 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*

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

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

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

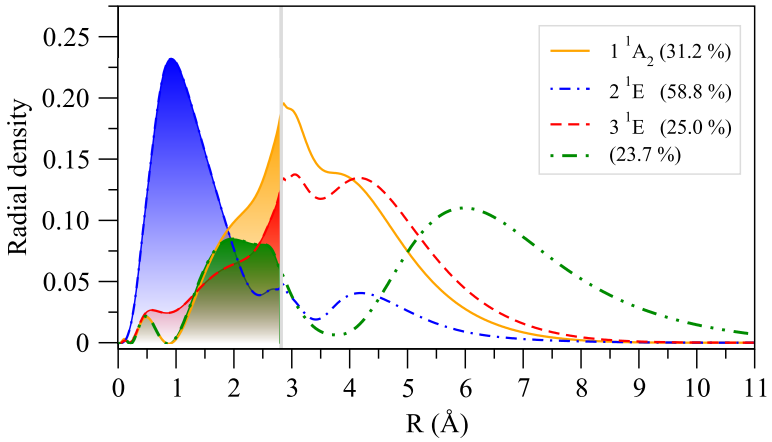

Figure 1: Radial density distributions of the singly-occupied natural orbitals occupied by the excited electron in the core excited states 3609.11 eV ($1\,^1A_2$), 3609.41 eV ($2\,^1E$) and 3609.64 eV ($3\,^1E$) of $K^+(H_2O)_6$. The grey line at 2.816 Å represents the equilibrium K-O distance.

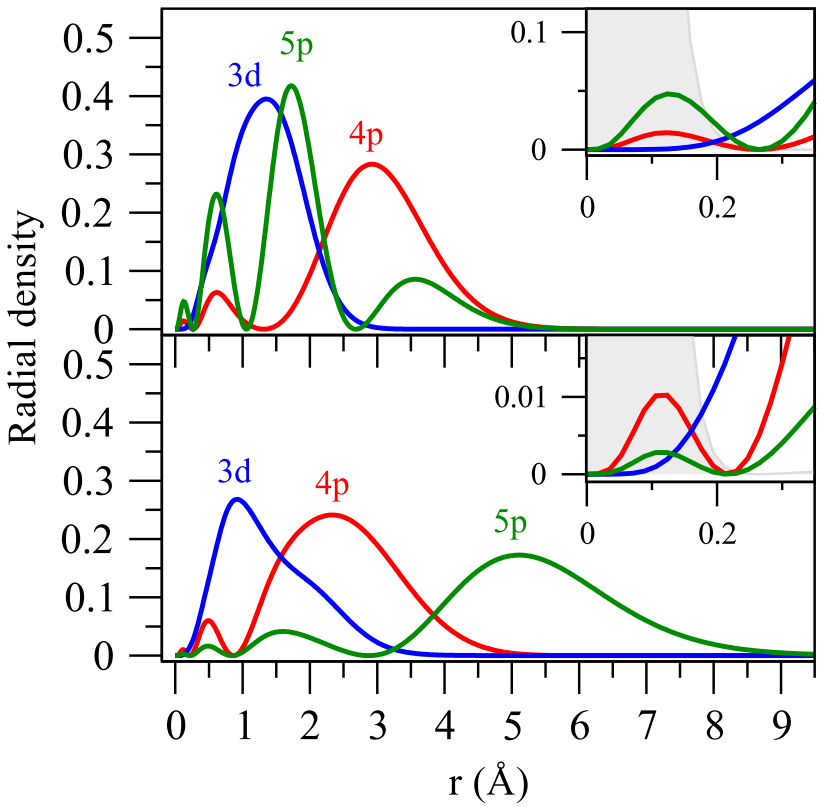

Figure 2: Radial density distributions of the singly-occupied natural orbital occupied by the excited electron corresponding to the 1s→4p, 1s→3d and 1s→5p core excitations in K^+ (lower panel) and Cl^- (upper panel). The insets show the region of distances relevant for the overlap with the 1s core orbital whose radial density is shown as a grey shaded area.