Water dipole orientation, Proton Transfer and Auger electron acceleration in Liquid water probed with Core-Level Spectroscopies

CARNIATO Stéphane

Laboratoire de Chimie-Physique Matière et Rayonnement (LCPMR), Sorbonne Université (SU), UMR 7614 du CNRS, 4 place Jussieu, Paris

The study of liquids using core-level spectroscopies is at the forefront of modern research, providing unique insight into electronic structure, solvation, and chemical interactions. In this work, we illustrate the power of these approaches through three representative examples. First, we will investigate aqueous Cu^{2+}, revealing [1] how X-ray photoelectron spectroscopy combined with simulations allows determination of the orientation of water dipoles in the first solvation shell of copper. Second, copper–glycine complexes are studied, showing proton transfer within the amino acid during complexation, and how this governs metal–ligand coordination, as evidenced by N 1s and Cu 2p spectra [2]. Finally, Auger electron acceleration effect in aqueous Ca^{2+} are highlighted through analysis and simulation of the Ca K-LL Auger spectrum [3]. Together, these examples demonstrate how core-level spectroscopy, combined with advanced modeling, provides detailed molecular-level understanding of solvation, coordination, and exotic electronic processes in liquids.

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