Fingerprint of the dipole orientation of water molecules in Cu^{2+} aqueous solution probed by x-ray photoelectron spectroscopy

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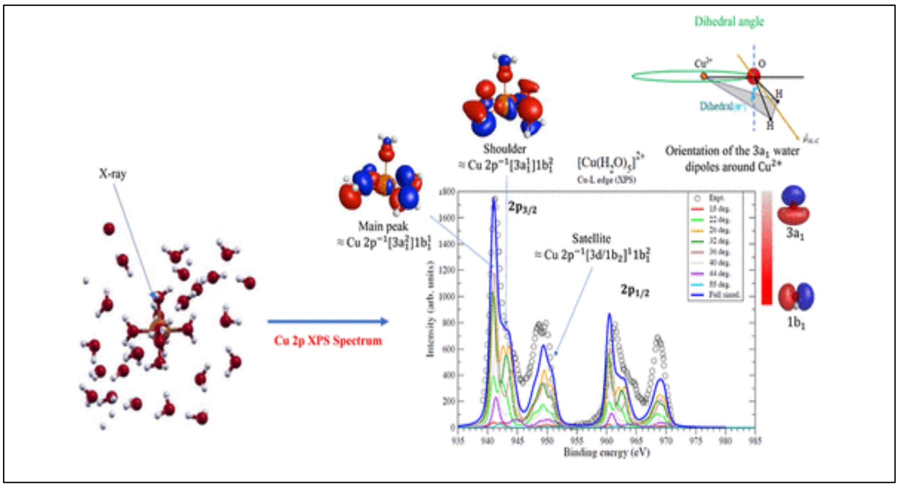
Keywords: liquid, X-ray photoelectron spectroscopy, ab-initio molecular dynamics and simulation of core-level spectra

The hydration of transition metals in aqueous solutions has long been studied due to its theoretical and experimental complexity, with much focus on the number of water molecules in the first coordination shell. Various methods, including EXAFS, NEXAFS, neutron diffraction, and computational approaches like Molecular Dynamics and Density Functional Theory, have been employed.

Recently, X-ray Photoelectron Spectroscopy (XPS) recorded the core-level spectra of copper compounds in liquid for the first time. Although typically used to identify chemical shifts and oxidation states, XPS has now been shown to reveal the orientation of neighboring water molecules through secondary excitations following Cu2p core ionization. This discovery highlights a novel use of XPS in probing non-covalently bonded systems, offering insights into dipole moment distributions. The ab-initio calculations of the Cu 2p core-level spectra presented in this context provide a comprehensive understanding of the underlying mechanisms responsible for both the main peak and satellite features.



[1] Mosaferi et al., *J. Am. Chem. Soc.* 2024, 146, 14, 9836-9850