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Ultrafast electron delocalization in aqueous L-cysteine

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Charge transfer (CT) processes play a fundamental role in chemistry and biomolecular interactions, particularly in aqueous environments where biological reactions occur. In this study, we utilize hard X-ray spectroscopy, specifically core-hole clock spectroscopy (CHCS), to probe ultrafast CT dynamics in L-cysteine solutions at different pH levels. The experimental setup involves high-resolution Auger electron spectroscopy at the SOLEIL and PETRA III synchrotrons, complemented by theoretical simulations to interpret the observed CT mechanisms.

Our results show that CT efficiency is strongly pH-dependent, with significant electron delocalization occurring in deprotonated L-cysteine at pH 12. This finding highlights the role of solvation, particularly the effects of the hydrogen-bonding network, in facilitating charge migration. The core-hole lifetime provides a natural timescale for electron transfer, enabling direct quantification of CT rates. Computational analysis further supports these trends, indicating that the electron transfer pathway is modulated by the protonation state of the thiol (-SH) and amino ($-NH_2$) functional groups.

Understanding CT in biomolecules is crucial for elucidating protein interactions, as well as for applications in fields such as radiation chemistry and environmental science. Our findings contribute to a deeper understanding of charge transport in solvated amino acids, paving the way for future research on complex biological molecules under X-ray irradiation.

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