CFEL SCIENCE

SEMINAR

8th November 2023 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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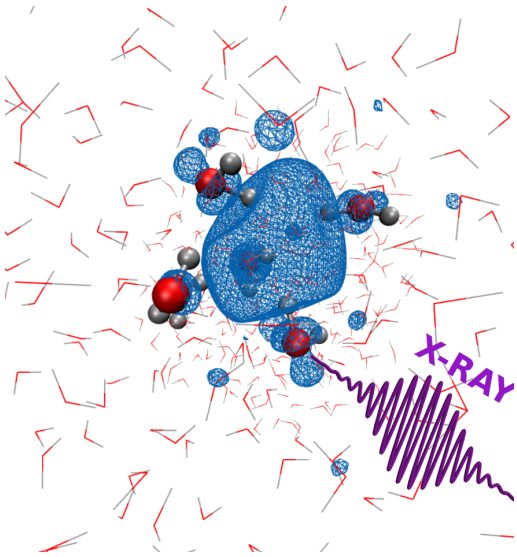
Tracking the birth of the electron solvation with X-rays



The attention that the solvated electron has received over the past half century, both from theory and experiment, is well justified due to its fundamental role in the chemistry of water. Its high reactivity and its role in radiation damage to DNA have important implications in physics, chemistry, and biology. Albeit the apparent simplicity of this system, a unified picture of the solvation process remains elusive. To overcome this challenge, one might need to go beyond standard optical techniques, which are unable to disentangle the vibrational and electronic response. In this study, we explore the capabilities of time-resolved x-ray absorption spectroscopy (XAS) as a new tool to investigate the ultrafast dynamics of the formation of the solvated electron. We used ring-polymer molecular dynamics together with a recently published neural network-based force field trained on MP2 electronic structure calculations to simulate the evolution of an excess electron placed in bulk water. For snapshots of the simulations, we have calculated the XAS using the *ab initio* electronic structure toolkit XMOLECULE. We then compare these results with experimental measurements obtained at LCLS. The data reveal that it is possible to trace the solvation dynamics of the electron in liquid water by inspecting distinct features in the time-resolved XAS. Our simulations also show that the solvation dynamics is governed by random structural fluctuations present in water. As a consequence, the solvation time is highly sensitive to temperature and to the specific way the electron is injected into water.

Host: Robin Santra – CFEL-DESY Theory Division