

Distinct transient structural rearrangement of ionized water revealed by XFEL X-ray pump X-ray probe experiment.

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Using X-ray free electron laser (XFEL) radiation to conduct an X-ray pump X-ray probe experiment, we studied strongly ionized water as part of our ongoing work on radiation damage [1]. After irradiance with a pump pulse with a nominal fluence of $\sim 5 \times 10^5$ J/cm², we observed for pump-probe delays of 75 fs and longer an unexpected structural rearrangement, exhibiting a characteristic length scale of ~ 9 Å. Simulations suggest that the experiment probes a superposition of ionized water in two distinct regimes. In the first, fluences expected at the X-ray focus create nearly completely ionized water, which as a result becomes effectively transparent to the probe [2]. In the second regime, out of focus pump radiation produces O¹⁺ and O²⁺ ions, which rearrange due to Coulombic repulsion over 10s of fs. Importantly, structural changes in the low fluence regime have implications for the design of two-pulse X-ray experiments that aim to study unperturbed liquid samples. Our simulations account for two key observations in the experimental data: the decrease in ambient water signal and an increase in low-angle X-ray scattering. They cannot, however, account for the experimentally observed 9 Å feature. A satisfactory account of this feature presents a new challenge for theory.

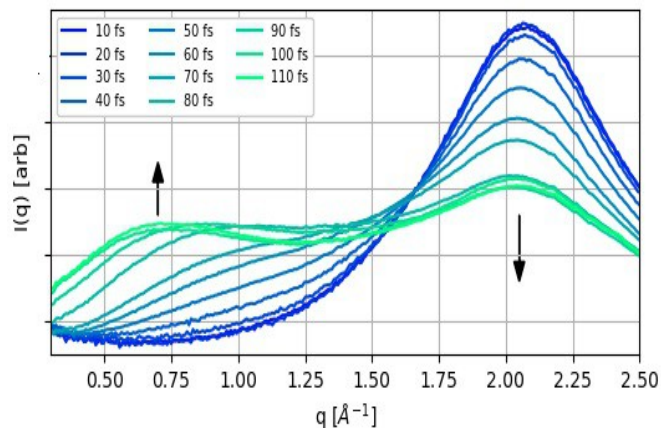


Figure 1. X-ray pump X-ray probe experiment reveals a new structural change in ionized water.

References

[1] M. Stransky, T. J. Lane, A. Gorel, S. Boutet, I. Schlichting, A. P. Mancuso, Z. Jurek, and B. Ziaja, *Commun. Phys.*, accepted, (2024).

[2] I. Inoue et al., *Phys. Rev. Lett.* **131**, 163201 (2023).

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