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Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics

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The dynamics of liquid water feature a variety of time scales, ranging from extremely fast ballistic-like thermal motion, to slower molecular diffusion and hydrogen-bond rearrangements. Here, will be presented our recent studies[1] using ultrafast coherent X-ray diffraction to investigate the sub-100fs dynamics of water from ambient conditions down to supercooled temperatures. This novel approach utilizes the inherent capability of X-ray speckle visibility spectroscopy at LCLS to measure equilibrium intermolecular dynamics with lengthscale selectivity, by measuring oxygen motion in momentum space.

The observed decay of the speckle contrast at the first diffraction peak, which reflects tetrahedral coordination, is attributed to motion on a molecular scale within the first 120 fs. Through comparison with molecular dynamics simulations, we conclude that the slowing down upon cooling from 328 K down to 253 K is not due to simple thermal ballistic-like motion, but that cage effects play an important role even on timescales over 25 fs due to hydrogen-bonding.

[1] F. Perakis et al., "Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics,"Nat. Commun., vol. 9, no. 1, p. 1917, (2018).

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