Abstract Submitted
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The hydrogen bond network of water supports propagating optical phonon-like modes[1] DANIEL ELTON, MARIVI FERNADEZ-SERRA, Stony Brook University — The local structure of liquid water as a function of temperature is a source of intense research. This structure is intimately linked to the dynamics of water molecules, which can be measured using Raman and infrared spectroscopies. Vibrational modes in liquids are usually considered to be associated to the motions of single molecules or small clusters. Previously, the librational Raman peaks of water were assigned to the librational motions of single molecules. By comparing experimental Raman and IR spectra we show these assignments are problematic. Using molecular dynamics simulations we study the k-dependent dielectric susceptibility of water. We find dispersive optical phonon-like modes in water's librational and OH stretching bands. We argue that on subpicosecond time scales these modes propagate through water's hydrogen bond network over distances of up to two nanometers. In the long wavelength limit these optical modes exhibit longitudinal-transverse splitting, indicating the presence of coherent long range dipole-dipole interactions. Studying how LO-TO splitting evolves with temperature may yield insight into how local structure changes. Our results indicate the dynamics of liquid water have more similarities to ice than previously thought. Reference: arXiv:1507.06363

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