

Abstract Submitted
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First principles calculation of the x-ray absorption spectra of ice and liquid water¹ DAVID PRENDERGAST², GIULIA GALLI³, Lawrence Livermore National Laboratory — Recent interpretations of x-ray absorption spectra (XAS) of ice and liquid water propose that the standard, tetrahedral model of the liquid should be replaced with a model where each water molecule possesses two stronger and two weaker hydrogen bonds to nearest neighbor molecules. We have investigated this issue and find no conclusive evidence to discount the standard model. Using density functional theory (DFT) calculations we find an excellent agreement with experiment for the XAS of ice I. We perform TIP4P classical molecular dynamics simulations of the liquid at 300K. Using 10 statistically uncorrelated snapshots of 32 molecules in our DFT calculations, we compute the XAS of this standard liquid model and also find a reasonable agreement with experiment. The spectral differences between liquid and solid arise from both structural disorder and the presence of dangling hydrogen bonds.

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