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Role of quantum nuclei and local fields in the x-ray absorption spectra of water and ice

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We calculate the x-ray absorption spectra of liquid water at ambient conditions and of hexagonal ice close to melting, using a static GW approach that includes approximately local field effects. Quantum dynamics of the nuclei is taken into account by averaging the absorption cross section over molecular configurations generated by path integral simulations. We find that inclusion of quantum disorder is essential to bring the calculated spectra in close agreement with experiment. In particular, the intensity of the pre-edge feature, a spectral signature of broken and distorted hydrogen bonds, is accurately reproduced, in water and ice, only when quantum nuclei are considered. The effect of the local fields is less important but non negligible, particularly in ice.

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