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Ab initio theory of X-ray emission spectral of liquid water

CHARLES SWARTZ, Temple University, SANTRA BISWAJIT, ROBERT DISTASIO, Princeton University, XIFAN WU, Temple University — X-ray emission spectral (XES) has recently been established as a powerful experimental tool in detecting the local H-bond network of liquid water. In the current work, we have developed an *ab initio* scheme for calculating the XES spectra of water. Based on the equilibrium trajectories generated by *ab initio* molecular dynamics, we perform additional atomic dynamics in the presence of a core-hole within the time scale corresponding to the experimental core-hole lifetime. The XES spectra is then determined by computing the transition matrix based on many body perturbation theory within the GW approximation. It is found that both the core-hole dynamics and the ensemble average of the local chemical environment, due to fluctuations of the H-bond network, are crucial in obtaining a physically meaningful XES spectra of liquid water.

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