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X-ray absorption spectra of ice and water: a first principles study with the GW method[1] XIFAN WU, WEI CHEN, ROBERTO CAR, Princeton University — We calculated the X-ray absorption spectra of ice and liquid water by adopting an approach based on the GW method to describe the excited electron in presence of a frozen core hole. We used the static Coulomb-hole and screened exchange approximation for the self-energy and used Maximally Localized Wannier functions to make GW calculations feasible in the large supercell needed to model a disordered system like water. The calculated spectra considerably improve the agreement with experiment, compared with previous DFT calculations. In particular, the three main features observed in experiments are well reproduced in terms of position and intensity for both ice and water. We also find that the difference between the ice and water spectra can be understood in terms of the electronic structures of these systems, manifested by a distorted, tetrahedral hydrogen bond network in the liquid.

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