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**Accurate prediction of x-ray absorption spectra using density functional theory**[1] GIULIA GALLI[2], DAVID PRENDERGAST[3], Lawrence Livermore National Laboratory — The increasing availability of x-ray absorption spectroscopy measurements for materials in the condensed phase is providing new opportunities to explore the local structure of disordered materials. However, the spectra produced by such experiments rely heavily on theoretical interpretation to infer the underlying atomic structure. We make use of density functional theory calculations to accurately approximate the initial and final state electronic structure associated with the absorption of an x-ray photon in the condensed phase. We outline some efficient computational approaches applied to ordered and disordered systems, concentrating on the K-edge absorption of oxygen. We report simulated x-ray absorption spectra for ice I, liquid water and magnesium oxide. Our results indicate excellent agreement with experiment for ice I and magnesium oxide, and our results for water, modelled using the classical TIP4P potential, indicate a reasonable qualitative agreement with experiment.

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[2]University of California, Davis
[3]University of California, Berkeley

David Prendergast
University of California, Berkeley

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