

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Ab initio study of near-edge x-ray absorption fine structure of hexagonal ice and liquid water WEI CHEN, Department of Physics, Princeton University, ROBERTO CAR, Department of Chemistry, Princeton University — We report first-principles calculations of near-edge x-ray absorption fine structure (NEXAFS) spectra of hexagonal ice and liquid water. Our work is motivated by the importance of accurately modeling NEXAFS spectra, which provide sensitive information on local molecular structures. In particular, we find a systematic improvement in the agreement of the calculated spectra with the experiment, by including excitonic effects, final state and self-interaction corrections. We correlate the calculated corrections to the degree of localization of the excited states.

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Date submitted: 24 Nov 2006

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