Abstract Submitted
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BSE/GW calculations of liquid and solid H_2O[1] JOHN VINSON, J.J. KAS, F.D. VILA, J.J. REHR, University of Washington, E.L. SHIRLEY, NIST, Gaithersburg MD — We have calculated both the UV/VIS and Oxygen K-edge x-ray spectra of model ice and water systems within many-body perturbation theory using state-of-the-art Bethe-Salpeter equation (BSE) and GW self-energy approximations [1], as implemented in the valence- and core-excitation codes OCEAN and AI2NBSE [2]. While the various phases of crystalline ice have well-characterized structures, the local environment and fluctuations of liquid water remain subjects of debate. Due in part to limitations of previous theoretical models, the interpretation of experimental probes has been controversial. We find that the BSE approach, which provides an accurate treatment of core-hole interactions, is vital for a quantitative agreement between experiment and theory. Likewise the effects of self-energy corrections within the GW approximation are needed to explain the observed band-stretching and damping of the spectra. Prospects for further improvements are briefly discussed.

[1] J. Vinson, J. J. Kas, F. D. Vila, J. J. Rehr, and E. L. Shirley, arXiv:1010.0025 (2011).
[2] J. Vinson et al., Phys. Rev. B 83, 115106 (2011); H. M. Lawler et al., Phys. Rev. B 78, 205108 (2008).

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