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Reconstructing the dynamical solvent structure around a model 'hydrated electron' using inelastic x-ray scattering R. CORIDAN, G.H. LAI, N. SCHMIDT, Dept of Physics, P. ABBAMONTE, Dept of Physics, Seitz Materials Research Lab, G.C.L. WONG, Depts of Mat. Science Eng. and Physics, and Seitz Materials Research Lab, U of Illinois, Urbana-Champaign, R. GODEWAT, S. GARDE, Dept of Chem and Bio Engineering, Rensselaer Polytechnic Institute, M. KRISCH, European Synchrotron Radiation Facility, A.Q.R. BARON, SPring-8/RIKEN and SPring-8/JASRI — The structure and dynamics of water on femtosecond timescales is relevant to many topics in physical chemistry such as electron solvation. We computationally reconstruct the Å-scale spatial and fs-scale temporal evolution of density fluctuations in water using high-resolution inelastic x-ray scattering (IXS). The imaginary part of density propagator χ(q,ω) is directly extracted from the IXS data, and the real part recovered using Kramers-Kronig relations. The resultant complex-valued χ(q,ω) is the Fourier transform of the real-space density-density response function χ(r,t) which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We use this density propagator and linear-response theory to reconstruct a model of the hydrated electron. The water density fluctuations as the electron 'diffuses' through bulk water can be observed. Moreover, preliminary data on the solvent response to changes in the electronic wave function will be presented.

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