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Reconstructing the dynamic hydration around hydrophobic molecular solutes using inelastic x-ray scattering R. CORIDAN, N. SCHMIDT, G.H. LAI, 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, M. MARUCHO, N. BAKER, Dept of Biochem. and Mol. Biophys., Center for Comp. Biology, Washington U School of Medicine — We combine inelastic x-ray scattering (IXS) data and liquid-state theory to image the dynamical hydration structure of water solvating molecular, hydrophobic solutes. Using 'linear response imaging', we computationally reconstruct the Å-scale spatial and fs-scale temporal evolution of density fluctuations in water using 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 density-density response function χ(r,t) which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We have shown that this propagator can be used to reconstruct the dynamical hydration around prototypical charge distributions. To extend this technique to more realistic solutes, Ornstein-Zernike integral equations from liquid state theory are used to study hydration around small excluded volumes. We will present results for simple geometries and discuss the implications of combining exclusion and charge.

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