

Is ambient water homogeneous or inhomogeneous?

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In a recent paper (PNAS, 2009, vol. 106, p.15214-15218) it is claimed structural heterogeneities have been observed in ambient water, based on small angle x-ray scattering (SAXS) and x-ray absorption and emission spectroscopies (XAS,XES). The evidence for this comes from two sources, namely the (small) rise in scattering at low wave vectors (Q) that occurs in the SAXS pattern for water, and the shapes of the XAS and XES spectra and the behaviour of these spectra with changing temperature. Using neutron and x-ray diffraction data and combining these with empirical potential structure refinement (EPSR) simulations, it is shown here that these claims are misconstrued, depending rather delicately on what exactly is meant by "inhomogeneous". The density fluctuations in water in the temperature range 0 - 100C are shown to have a single mode, do not exhibit the two (or more) mode structure that might be implied by the inhomogeneous model, and are more than sufficient to explain the low Q rise in the small angle x-ray scattering. It is also shown that current interpretations of XAS data from water using theoretical techniques are highly variable, and an alternative, evidence based, interpretation is proposed.