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The structure of water in bulk and in confinement by total neutron and x-ray scattering

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In the past decade or so there has been a significant worldwide effort to try to obtain a consistent set of radial distribution functions for water. Exactly how those distribution functions should be interpreted in terms of the local order in water remains a somewhat open question – whether for instance they imply water has a degree of heterogeneity in its local structure or whether it is in fact a uniform fluid with normal statistical fluctuations in density and structure. However combining a number of different x-ray and neutron data sets together is now indicating a rather consistent view of the local distribution functions in water. This consistency is achieved partly as a result of different researchers applying state-of-the-art data analysis methods to their data, both neutron and x-ray, but partly also by the application of computer simulation methods of structure refinement which help to eliminate some of the artifacts that can be introduced by uncertainties in that data analysis. The situation as regards confined water is much less clear. However it is possible to investigate water near a surface using radiation total scattering methods in the case where the pores which contain the water, whether sheet-like, cylindrical, or spherical, have a regular arrangement in the material. This is because the Bragg peaks arising from that regular arrangement are strongly affected depending on how the fluid is distributed within the pore. This talk will focus on the MCM41 silicas which have cylindrical pores on a hexagonal lattice. Combining the scattering data with computer structure refinement in the same way that is done for the bulk liquid is leading to unprecedented insight into how water is organized near the silicate surface. This work is aimed at clarifying the underlying processes that may have lead to recent observations of fragile to strong transitions in these materials.