

Is there a minimum density in confined water?

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To what extent it is possible to compare the microscopic structure of water confined in nanopores with that of bulk water? Here we use neutron diffraction experiments with isotopic substitution, coupled to coarse graining calculations and atomistic simulations, to investigate water confined in a silica matrix (MCM41-S-15). This comparison is made at 300 K and at 210 K, addressing, in particular, the issue related to the existence of a minimum of density at 210 K, as recently claimed.

The presence of hydrophilic pore surface causes a non homogeneous distribution of water molecules across the pore. As a consequence, we find a clear water density profile, with a layer of higher density near the pore surface and a region of lower density in the pore center. This non uniform pore occupancy is accompanied by sensible changes of the microscopic structure of water compared to bulk, here evidenced by a layer analysis of the site-site radial distribution functions.