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Topological cluster structure of water confined in hydrophobic pores

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In this study, we show the anomalous temperature dependence of the water density confined in hydrophobic sub-nanometer spaces from in situ XRD measurements [3], and computational analysis, hybrid reverse Monte Carlo simulation (HRMC) and the persistent homology method. The persistent homology method provides geometric intermolecular structural information about disordered materials, such as amorphous and liquid materials. In sub-nanometer spaces, the density of confined water is very sparse compared to that of bulk ice even at room temperature, suggesting that the spatially distorted ice-like hydrogen bonding network would be formed in the nanospaces.

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