NANODROPLETS AND THE EQUATION OF STATE OF DEEPLY SUPERCOOLED WATER

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We carry out extensive molecular dynamics simulations of nanoscale liquid droplets of the TIP4P/2005 model of water, with number of molecules ranging from N = 64 to 2880 and temperatures down to 180 K. As droplet size decreases, the Laplace pressure induced by the liquid-vapour surface tension increases. For sufficiently small droplets, the density within droplets exceeds the critical density associated with the liquid-liquid critical point proposed to occur deep in the supercooled region of the model. Since crystallization is suppressed for such small droplets, they provide a possible experimental probe for determining the equation of state for water where crystallization is otherwise unavoidable, and hence could provide direct evidence for the much-investigated second critical point scenario. However, it is unclear whether such small systems can provide any information on bulk water. We report on our progress in determining the relationships between N, temperature, pressure, and density, including the emergence of anomalous behaviour emblematic of bulk liquid water.