

# Ice nucleation near the fragile-to-strong crossover in simulations of supercooled water

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## **Abstract:**

Recent free energy simulations of supercooled water using the ST2 potential have confirmed the existence of a liquid-liquid phase transition (LLPT) in this water model. However, the influence of the LLPT on the nucleation of ice in this model has not been quantified, in particular, the influence on the height of the nucleation barrier. To address this question, we carry out umbrella sampling Monte Carlo simulations of ST2 water to evaluate the free energy of formation of small sub-critical clusters of ice Ic. We estimate this free energy over a range of temperature and pressure in the supercooled region of the phase diagram straddling the so-called Widom line, which is associated with a fragile-to-strong crossover in the dynamical behavior of the liquid. Our results demonstrate that the supercooled liquid phase in this regime is separated from the ice phase by a substantial free energy barrier. We also reveal a crossover in the behavior of the free energy of formation of small ice clusters as the liquid moves from the high density to the low density regime.