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Liquid-liquid transition in the ST2 model of water

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We present clear evidence of the existence of a metastable liquid-liquid phase transition in the ST2 model of water. Using four different techniques (the weighted histogram analysis method with single-particle moves, well-tempered metadynamics with single-particle moves, weighted histograms with parallel tempering and collective particle moves, and conventional molecular dynamics), we calculate the free energy surface over a range of thermodynamic conditions, we perform a finite size scaling analysis for the free energy barrier between the coexisting liquid phases, we demonstrate the attainment of diffusive behavior, and we perform stringent thermodynamic consistency checks. The results provide conclusive evidence of a first-order liquid-liquid transition. We also show that structural equilibration in the sluggish low-density phase is attained over the time scale of our simulations, and that crystallization times are significantly longer than structural equilibration, even under deeply supercooled conditions. We place our results in the context of the theory of metastability.