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Evaluating the Liquid Liquid Phase Transition Hypothesis of Supercoooled Water DAVID LIMMER, DAVID CHANDLER, University of California, Berkeley — To explain the anomalous behavior of supercooled water it has been conjectured that buried within an experimentally inaccessible region of liquid water's phase diagram there exists a second critical point, which is the terminus of a first order transition line between two distinct liquid phases. The so-called liquid-liquid phase transition (LLPT) has since generated much study, though to date there is no consensus on its existence. In this talk, we will discuss our efforts to systematically study the metastable phase diagram of supercooled water through computer simulation. By employing importance-sampling techniques, we have calculated free energies as a function of the density and long-range order to determine unambiguously if two distinct liquid phases exist. We will argue that, contrary to the LLPT hypothesis, the observed phenomenology can be understood as a consequence of the limit of stability of the liquid far away from coexistence. Our results suggest that homogeneous nucleation is the cause of the increased fluctuations present upon supercooling. Further we will show how this understanding can be extended to explain experimental observations of hysteresis in confined supercooled water systems.

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