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The Putative Liquid-Liquid Transition is a Liquid-Solid Transition in Atomistic Models of Water DAVID CHANDLER, DAVID LIMMER, Department of Chemistry, University of California, Berkeley — Our detailed and controlled studies of free energy surfaces for models of water find no evidence for reversible polyamorphism, and a general theoretical analysis of the phase behavior of cold water in nano pores shows that measured behaviors of these systems reflect surface modulation and dynamics of ice, not a liquid-liquid critical point. A few workers reach different conclusions, reporting evidence of a liquid-liquid critical point in computer simulations of supercooled water. In some cases, it appears that these contrary results are based upon simulation algorithms that are inconsistent with principles of statistical mechanics, such as using barostats that do not reproduce the correct distribution of volume fluctuations. In other cases, the results appear to be associated with difficulty equilibrating the supercooled material and mistaking metastability for coarsening of the ordered ice phase. In this case, sufficient information is available for us to reproduce the contrary results and to establish that they are artifacts of finite time sampling. This finding leads us to the conclusion that two distinct, reversible liquid phases do not exist in models of supercooled water.

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