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**Metastable liquid-liquid phase separation and criticality in water-like models** RAKESH SINGH, Princeton University, JOHN BIDDLE, University of Maryland, PABLO DEBENEDETTI, Princeton University, MIKHAIL ANISIMOV, University of Maryland — Water shows intriguing thermodynamic and dynamic anomalies in the supercooled liquid state. A possible explanation of the origin of these anomalies lies in the existence of a metastable first order liquid-liquid phase transition (LLPT) between two (high and low density) forms of liquid water. Unambiguous experimental proof of existence of LLPT in bulk supercooled water is so far hampered by ultra-fast ice crystallization. Computer simulations of water models are therefore crucial for exploring the possibility of LLPT in deeply supercooled water. We present computer simulation results that elucidate the possibility of a metastable LLPT in one of the most accurate atomistic models of water, TIP4P/2005. To describe the computed properties, we have applied two-state thermodynamics, viewing water as a non-ideal mixture of two inter-convertible states. The thermodynamic behavior of the model in the one-phase region suggests the existence of energy-driven LLPT. We compare the behavior of TIP4P/2005 with other popular water models, and with real water, all of which are well-described by two-state thermodynamics. Additionally, we also elucidate the relation between the phenomenological order parameter of the two-state thermodynamics and the microscopic nature of the low-density structure.

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