

Abstract Submitted  
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**Liquid-liquid coexistence and crystallization in supercooled ST2 water**<sup>1</sup> FAUSTO MARTELLI, Department of Chemistry, Princeton University, JEREMY PALMER, PABLO DEBENEDETTI, Department of Chemical and Biological Engineering, Princeton University, ROBERTO CAR, Department of Chemistry, Princeton University — We have computed the free energy landscape of ST2 water in the supercooled regime (228.6 K and 2.4 kbar) using several state-of-the-art computational techniques, including umbrella sampling and metadynamics. Such results conclusively demonstrate coexistence between two liquid phases, a high-density liquid (HDL) and a low-density liquid (LDL), which are metastable with respect to cubic ice. We show that the three phases have distinct structural features characterized by the local structure index and ring statistics. We also find that ice nucleation, should it occur, does so from the low-density liquid. Interestingly, we find that the number of 6-member rings increases monotonically along the path from HDL to LDL, while non-monotonic behavior is observed near the saddle point along the LDL-ice I<sub>c</sub> path. This behavior indicates a complex re-arrangement of the H-bond network, followed by progressive crystallization.

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