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Amorphous ices explained in terms of nonequilibrium phase transitions in supercooled water DAVID LIMMER, DAVID CHANDLER, Department of Chemistry, University of California, Berkeley — We analyze the phase diagram of supercooled water out-of-equilibrium using concepts from space-time thermodynamics and the dynamic facilitation theory of the glass transition, together with molecular dynamics simulations. We find that when water is driven out-of-equilibrium, it can exist in multiple amorphous states. In contrast, we find that when water is at equilibrium, it can exist in only one liquid state. The amorphous non-equilibrium states are solids, distinguished from the liquid by their lack of mobility, and distinguished from each other by their different densities and local structure. This finding explains the experimentally observed polyamorphism of water as a class of nonequilibrium phenomena involving glasses of different densities. While the amorphous solids can be long lived, they are thermodynamically unstable. When allowed to relax to equilibrium, they crystallize with pathways that pass first through liquid state configurations and then to ordered ice.

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