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Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water

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Most liquids can form a single glass or amorphous state when cooled sufficiently fast (in order to prevent crystallization). However, there are a few substances that are relevant to scientific and technological applications which can exist in at least two different amorphous states, a property known as polyamorphism. Examples include silicon, silica, and in particular, water. In the case of water, experiments show the existence of a low-density (LDA) and high-density (HDA) amorphous ice that are separated by a dramatic, first-order like phase transition. It has been argued that the LDA-HDA transformation evolves into a first-order liquid-liquid phase transition (LLPT) at temperatures above the glass transition temperature Tg. However, obtaining direct experimental evidence of the LLPT has been challenging since the LLPT occurs at conditions where water rapidly crystallizes. In this talk, I will (i) discuss the general phenomenology of polyamorphism in water and its implications, and (ii) explore the effects of a LLPT on the pressure dependence of Tg(P) for LDA and HDA. Our study is based on computer simulations of two water models – one with a LLPT (ST2 model), and one without (SPC/E model). In the absence of a LLPT, Tg(P) for all glasses nearly coincide. Instead, when there is a LLPT, different glasses exhibit dramatically different Tg(P) loci which are directly linked with the LLPT. Available experimental data for Tg(P) are only consistent with the scenario that includes a LLPT (ST2 model) and hence, our results support the view that a LLPT may exist for the case of water.