Physics
AT QUEENS COLLEGE

Colloquium Notice

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

Most liquids can form a single glass or amorphous state when cooled fast enough, so crystallization is avoided. However, there are a few substances that are relevant to scientific and technological applications that 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 connects to a first-order liquid-liquid phase transition (LLPT) above the glass transition temperature Tg. However, direct experimental evidence of the LLPT is challenging to obtain, since the LLPT occurs at conditions where water rapidly crystallizes. In this work, we (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 LLCP may exist for the case of water.

Monday
September 10, 2012
Starts at 12:15 PM
Coffee at 12:00 PM
Physics Conference Room, SB B326