Abstract Submitted
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Polyamorphism in Tetrahedral Liquids[1] JEREMY PALMER, Univ of Houston — Tetrahedral liquids exhibit well-known thermophysical anomalies that arise from a competition between high-density and low-density local coordination structures in the fluid. These structures allow such systems to form both high-density and low-density glassy phases upon rapid cooling. It has been posited that these experimentally observed glass phases are associated with two distinct ergodic liquids at higher temperatures that undergo a first-order liquid-liquid phase transition (LLPT). Direct experimental observation of these hypothesized LLPTs, however, has proved to be challenging because they are typically predicted to occur at conditions where the liquids are metastable with respect to crystallization. Here, we discuss recent computational studies of model tetrahedral liquids that exhibit metastable LLPTs. Using free energy analysis, we show that the ST2 water model, the TIP5P water model, and an ionic model of silica exhibit LLPTs under deeply supercooled conditions. We investigate the nature of the LLPTs in these systems and show that liquid-liquid phase separation can be observed in large-scale molecular dynamics simulations. Finally, we investigate nucleation of the stable crystal phase and demonstrate that this process is distinct from those involved in LLPTs.

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