

The effect of attractive interaction on the thermodynamic fragility

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Abstract:

In this talk we will present a comparative study of the dynamic and thermodynamic properties of Binary Lennard-Jones (LJ) and the corresponding Weeks-Chandler-Anderson (WCA) mixtures. Berthier and Tarjus in a series of paper have shown that although the two systems have similar pair structure but in the viscous liquid regime their dynamics are widely different [1-4]. The kinetic fragility of the LJ system is larger than the WCA system. We show that although the pair structures of the two models are apparently very similar, which would ideally imply that the thermodynamic properties are also similar, they significantly differ in their thermodynamic fragility. The difference in the thermodynamic fragility and also the difference in their high temperature behaviour together can account for the difference in their kinetic fragility. Coslovich has shown that although the pair structures of the two models are close but at the level of higher order correlations they are different [5]. Thus it can be argued that the many body contribution to the entropy leads to the large difference in the thermodynamic fragility. However, we show that not only the multiple particle entropy but also the entropy obtained from only the pair contribution are widely different for the two systems.

References:

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