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Computer simulation of structure and dynamics of liquids¹

THOMAS TRUSKETT, University of Texas at Austin

In this talk, I will discuss some of what recent computer simulation studies have taught us about the relationship between the real-space structure and dynamics of model equilibrium and supercooled fluids. Specifically, I will discuss which experimentally measurable aspects of static structure reliably track the dynamical trends of homogeneous and confined equilibrium fluids, and which do not. I will also explain how some of the well-known “dynamic anomalies” of supercooled water and concentrated suspensions of particles with short-range attractions, reflect corresponding anomalies in the underlying static structure. Finally, I will explore how dynamic heterogeneities of deeply supercooled fluids connect to dynamic aspects of their local structure.

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