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Is there a connection between structure and heterogeneous dynamics in supercooled liquids? WILLIAM KREKELBERG, VENKAT GANESAN, THOMAS TRUSKETT, University of Texas-Austin, Department of Chemical Engineering — Structurally arrested (jammed or glassy) states are often prepared from supercooled fluids, though there a number of open questions regarding how that process occurs. One involves explaining why modest increases in structural order accompany the pronounced slowing of liquid-state dynamics near structural arrest. Another involves understanding why self-diffusion in deeply supercooled fluids occurs much faster than would be predicted from knowledge of the viscosity and the Stokes-Einstein relation. Single-particle displacements become heterogeneous near the glass transition, but corresponding structural heterogeneities have been difficult to identify. Collectively, these observations call into question the general prospect of understanding and predicting dynamical behavior of liquids based on structural information. In this talk, we present simulation data on several model systems that show that the dynamics of supercooled liquids can be quantitatively correlated to structure in a simple way. Specifically, we show that the breakdown of the Stokes-Einstein relationship reflects simple and distinct couplings between structure, viscosity, and diffusivity in the supercooled fluid. We also demonstrate how heterogeneous dynamics correlate with dynamically heterogeneous structure.

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