Shedding light on collective dynamics in supercooled liquids with the isoconfigurational ensemble: exploring structure-dynamics correlations

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Abstract

Glasses - formed via a continuous transition from the liquid to the solid state - are ubiquitous in nature and play an important role in many technological applications, yet we still lack a clear picture of the relationship between structure and dynamics in such materials. For example, the role of structure in the appearance of slowly relaxing domains whose dimensions and lifetimes increase with supercooling.

In this talk, I will present the isoconfigurational ensemble as a useful general tool for exploring the relationship between structure and dynamics when order is ill-defined and transient. In particular, I will show that as supercooling increases, a given configuration increasingly constrains the propensity of particles to subsequently exhibit large displacements. This dynamic propensity allows one to test various hypotheses about the causal relationship between structure and dynamics at a microscopic level, and to ultimately arrive at a measure of structure that correlates with the spatial variation in propensity. I will also briefly discuss some of the other questions that can be addressed using the isoconfigurational ensemble.

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