New Methods for Computing the Configurational Entropy of Deeply Supercooled Liquids with the Potential Energy Landscape

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Quantifying the nonexponential relaxation of supercooled liquids in terms of thermodynamics is a major open question in physical chemistry. The Adam-Gibbs model expresses the relaxation time, a kinetic property, in terms of the configurational entropy, a thermodynamic property. However, it is difficult to accurately determine the configurational entropy through thermodynamic experiments, because doing so requires measuring the translational, vibrational, and rotational contributions to the isobaric heat capacity with minimal error. My research addresses this problem by formulating three important results regarding the low-temperature behavior of supercooled liquids. First, I use statistical mechanics to evaluate the isobaric enumeration function of five glass-forming liquids that span a wide range of fragilities. Second, I develop a diffusion model to obtain a relationship between the self-diffusion coefficient and the configurational entropy, which is the fraction of the entropy that only depends on particle configurations. My diffusion model provides a direct method to determine the configurational entropy through experimental measurements. Third, I establish a link between the stretched exponential parameter and the configurational fraction, defined as the ratio of the configurational entropy to the excess entropy of the supercooled liquid over the crystal. I use this link to predict configurational fractions for the five glass-forming liquids. This work makes important progress on the open problem and advances the fundamental understanding of supercooled liquids, allowing for the meaningful exploration of their applications such as nuclear waste storage and drug delivery.

Awards Won:
YM American Academy: Third Award of $500.00