Microscopic dynamics and thermodynamics on a dipolar glass former

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Abstract

Free energy and entropy have been evaluated for a supercooled dipolar model liquid, and their connections with structure and dynamics on the supercooled state have been explored by using perturbative calculations, molecular dynamics simulations and instantaneous normal mode analysis. A model is proposed in order to analyze translation and rotation contributions to entropy separately. The approach states that both of them contain gas-like and solid-like terms. Results are consistent with a preferential intrabasin energy landscape dynamics in the supercooled state. A logarithmic correlation between excess entropy associated with translation and the corresponding imaginary modes is encountered. Rosenfeld scaling law between reduced diffusion and excess entropy is tested, and it is obtained that it is valid within the same temperature range as the Arrhenius law for diffusion. The microscopic origin of the breakdown of Rosenfeld scaling at low temperatures is investigated and it results from an increasing relevance of mode-coupling contributions to diffusion.

References:

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