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Contribution ID: **286** Type: **Poster Competition (Graduate Student) / Compétition affiches (Étudiant(e) 2e ou 3e cycle)**

(POS-18) A molecular dynamics simulation study of glassy dynamics in supercooled glycerol.

Tuesday 10 June 2025 18:00 (2 minutes)

Glycerol is a well-known molecular glass former that appears in several natural and engineered systems and has applications in cryopreservation, amorphous drug formulations, and stabilization of biomolecules. As it is cooled, the viscosity and structural relaxation time, of the liquid rapidly increase until the system falls out of metastable equilibrium and becomes trapped in an amorphous solid state at the glass transition temperature. However, little is known about how the structure of the liquid influences its dynamics. In this work, we use molecular simulation to explore the relationships between structure and dynamics, with a focus on understanding the nature of structural and dynamic heterogeneity in this molecular glass former. The glass transition temperature of the system is determined from the temperature dependence of the density and heat capacity. The dynamics of the system are measured and studied by measuring the diffusion coefficients and neighbour structural relaxation times, while the local dynamics associated with conformational changes are measured in terms of the dihedral angle rotational correlation function. Finally, dynamic heterogeneity is studied using the iso-configurational neighbour relaxation time for individual molecules.

Keyword-1

Dynamic heterogeneity

Keyword-2

Relaxation time

Keyword-3

Structural heterogenity

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