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**Insights into Polymer Normal Mode Dynamics During Glass formation from Efficient In-Equilibrium Molecular Dynamics Simulation**[1]
JUI-HSIANG HUNG, TARAK PATRA, JAYACHANDRA HARI MANGARALA, DAVID SIMMONS, The University of Akron — The Rouse model of chain dynamics is the foundational model for the normal mode dy-namics of unentangled polymer melts. A central prediction of this model is that the tem-perature dependence of a chain's normal mode relaxation time is coupled to the tempera-ture dependence of its segmental relaxation time. However, studies of polymers near their glass transition temperature Tg have sometimes observed a failure of this coupling. Most commonly, end-to-end dynamics and viscosity are observed to exhibit a weaker tempera-ture dependence than segmental dynamics in this temperature range, signaling a break-down in time-temperature superposition. Here we describe long-time molecular dynamics simulations of chain normal mode dynamics in the supercooled regime. Results indicate that a decoupling of chain normal modes leads to an incipient 'crisis' at which whole chain relaxation is extrapolated to occur more rapidly than segmental relaxation at tempera-tures below Tg. We compare this behavior to the predictions of several established models of glass formation in order to elucidate its physical origins.

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