

~~Special Polymer Physics Seminar ~~

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**10:00 AM Tuesday,
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301 Steidle Bldg.**

Influence of Nanoparticles on Fragility and Collective Particle Motion in Polymer Glass-Formation

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We investigate the impact of nanoparticles (NP) on glass-formation in polymer melts by molecular dynamics simulation. The NP cause significant changes in both fragility and the average length L of string-like cooperative motion, where the extent of the effect depends on the NP-polymer interaction and NP concentration. These dynamical changes can be interpreted via the Adam-Gibbs (AG) theory if we assume the strings represent the abstract “cooperatively rearranging regions” of the AG model, whose basic assumptions are reviewed. Molecular additives are also effective at altering the fragility of glass-formation and extent of string-like collective motion so the modulation of fragility and cooperative motion with additives seems to be a general effect. We find that the fragility of glass formation is mainly controlled by the differential change of L with respect to T near the glass transition rather than the actual size L of the collective motion. We also find a near proportionality between m and T_g in our nanocomposite system, as found for high molecular mass polymers and we note that this greatly simplifies the T dependence of structural relaxation in restricted classes of materials where this scaling relation holds. The classical entropy theory of glass-formation is considered as a complementary tool to gain analytic insights into these additive effects on polymer glass formation.