Supporting information for article:

Atomistic Molecular Insight into the Time Dependence of Polymer Glass Transition

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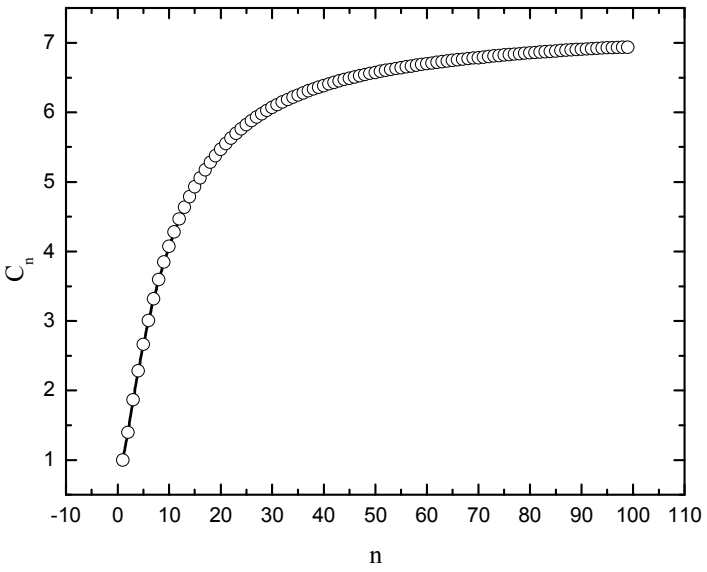

Figure 1s. Polymer characteristic ratios averaged over all chain segments along the backbone of the linear polymer chains.

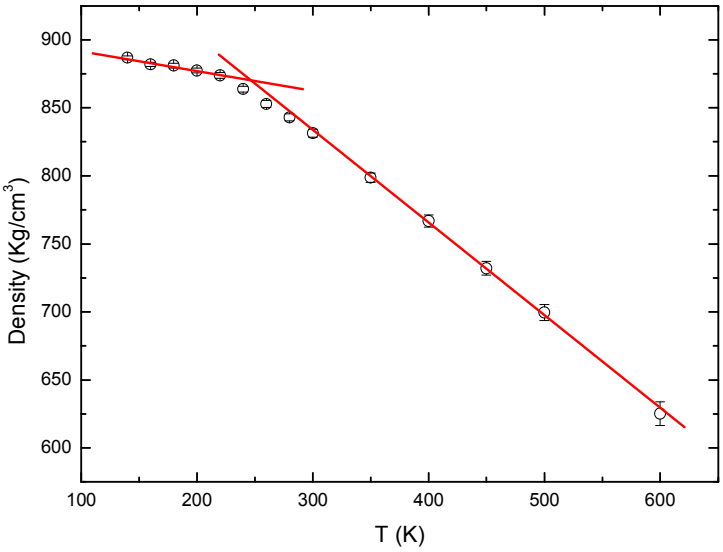

Figure 2s. Average densities of the systems during the production runs and the error bars show the standard deviations; the solid lines are linear fits, whose intersection around 250 K gives the volumetric glass transition.

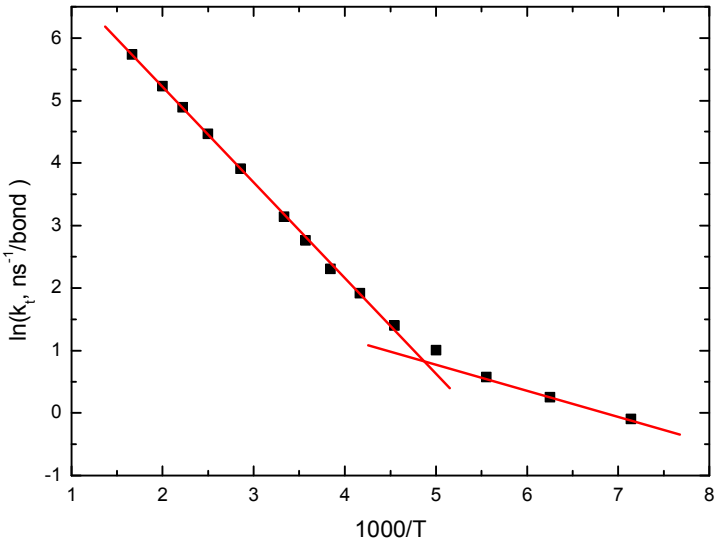

Figure 3s. The logarithmic overall conformational transition rates plotted with inverse temperature; the solid lines are linear fits, whose intersection around 206 K gives the microscopic glass transition, which was also discussed in our previous paper (J. Phys. Chem. B 2009, 113, 9077-9083).

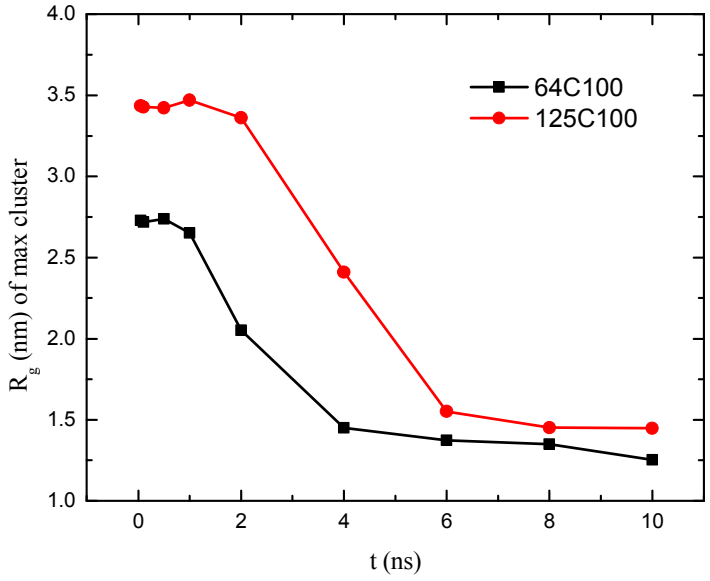

Figure 4s. Variation of the max cluster size at the same temperature of 200 K for $125C_{100}H_{202}$ and $64C_{100}H_{202,}$ whose system sizes are around 7.0 nm and 5.5 nm respectively. The frozen torsions obtained within smaller observation times in both systems formed volume spanning frozen clusters.