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Molecular dynamics simulations on mid-linked polymer matrix ADAM DILLON, HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, DEVESH MISRA, Department of Chemical Engineering, University of Louisiana at Lafayette — We utilize molecular dynamics simulations to probe the dependence of thermodynamic properties on the structure of polymer molecules. We study four different polymer materials: (1) Long chain polymers of ~50 united atoms, (2) short chain polymers of ~10 united atoms, (3) mixture of long and short chain polymers with varied mixing ratio, and (4) polymer matrix of Long chains cross-linked by short chains. Here the cross-linking sites are not at the end of the chain (end-linked) of which most previous studies were done, but in the middle of the chain (mid-linked). We will discuss the difference in thermodynamic properties, such as glass transition temperature, among these four structures.

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