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Unconcatenated ring polymer melts: Molecular dynamics study of the static and dynamic properties JONATHAN HALVERSON, MPI for Polymer Research, WON BO LEE, GARY GREST, ALEXANDER GROSBERG, KURT KREMER — Molecular dynamics simulations were conducted to investigate the dynamic and structural properties of unconcatenated ring polymer melts in comparison to linear polymer melts. Systems were composed of 200–2500 polymer chains at a reduced temperature and density of 1.0 ϵ and 0.85 σ^{-3}, respectively. With N denoting the number of monomers per chain, simulations were conducted with N = 100, 200, 400 and 800. For the ring polymers an additional simulation was conducted with N = 1600. The standard polymer melt model was modified by introducing a bending potential to make the chains stiffer. For each value of N, the ring polymers were found to have a higher diffusivity than their linear counterparts. While the ring polymers are found to be roughly spherical in shape, they display complex dynamic correlations as revealed by a primitive path analysis.

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