



سمینار هفتگی ماده چگال نرم

Journal Club:

Thermodynamics and Structure of Poly[n]catenane Melts

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Macromolecules

Abstract

Motivated by recent achievements in the synthesis of interlocking polymers, the structural features of poly[n]catenanes, polymers composed entirely of interlocking rings (or macrocycles), are studied by extensive molecular dynamics simulations in the melt state. The degree of polymerization (number of links) is varied from $n = 1-25$ and the number of beads per macrocycle is varied from $m = 15-50$; the results are compared to linear chains of degrees of polymerization $N = 15-175$. The mechanical bonds in the system cause significant topological contributions to the pressure and potential energy density not seen in other polymer systems. The polymers themselves possess many unusual structural features at short and intermediate length scales, which can be attributed to density inhomogeneities along the polymer contour. Furthermore, the conformations of the individual macrocycles within poly[n]catenanes are quite different from those of ordinary ring polymers and depend on the topology of the macrocycle, that is, whether it is threaded by one ring (chain end) or two (chain center). At larger length scales, the poly[n]catenanes are conformationally similar to ideal linear chains, but unlike traditional (covalent) polymers, they are highly globular at low degrees of polymerization and are extremely flexible relative to their size, which inhibits interchain entanglement. Implications for poly[n]catenane material properties and synthesis are discussed.

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