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Predicting χ for polymers with stiffness mismatch from simulations DANIEL KOZUCH, WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Department of Chemical Engineering, Penn State University — The Flory-Huggins χ parameter describes the excess free energy of mixing and governs phase behavior for polymer blends and block copolymers. For chemically distinct polymers, the value of χ is dominated by the mismatch in cohesive energy densities of the monomers. For blends of chemically similar polymers, the entropic portion of χ, arising from non-ideal local packing, becomes more significant. Using polymer field theory, Fredrickson, Liu, and Bates predict that a difference in backbone stiffness can result in a positive χ for chains consisting of chemically identical monomers. To quantitatively investigate this phenomenon, we perform molecular dynamic (MD) simulations for bead-spring chains which differ only in stiffness. From the simulations, we apply a novel thermodynamic integration to extract χ as low as 10^{-3} per monomer for blends with mild stiffness mismatch. By introducing a standardized effective monomer, we map real polymers to our bead-spring chains and show that the predicted entropic portion of χ are consistent with experimental data.

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