MAR17-2016-000389

Configurations and Dynamics of Semi-Flexible Polymers in Good and Poor Solvents

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We develop coarse-graining procedures for determining the conformational and dynamic behavior of semi-flexible chains with and without flow using Brownian dynamics (BD) simulations that are insensitive to the degree of coarse-graining. In the absence of flow, in a poor solvent, we find three main collapsed states: torus, bundle, and globule over a range of dimensionless ratios of the three energy parameters, namely solvent-polymer surface energy, energy of polymer folds, and polymer bending energy or persistence length. A theoretical phase diagram, confirmed by BD simulations, captures the general phase behavior of a single long chain (>10 Kuhn lengths) at moderately high (order unity) dimensionless temperature, which is the ratio of thermal energy to the attractive interaction between neighboring monomers. We also find converged results for polymer conformations in shear or extensional flow in solvents of various qualities and determine scaling laws for chain dimensions for low, moderate, and high Weissenberg numbers Wi. We also derive scaling laws to describe chains dimensions and tumbling rates in these regimes.