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Effects of Bond Stiffness on Structural Transitions of Flexible Polymers TOMAS KOČI, MICHAEL BACHMANN, Center for Simulational Physics University of Georgia — Utilizing advanced parallel Monte Carlo simulation methods we examine the structural transitions of a coarse-grained flexible polymer model. In this model, the bond elasticity or effective bond stiffness is considered to be a parameter. Pseudophase diagrams in temperature-stiffness space are constructed by using energy dependent canonical quantities to demonstrate the effects of the changes in the bond flexibility on the liquid and solid structural phases. With increasing bond flexibility we observe the disappearance of the liquid phase and the fusion of the collapse and the freezing transitions. The notoriously difficult sampling of entropically suppressed energetic regions near strong first-order transitions is improved by employing generalized ensemble methods.

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