

Abstract Submitted  
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**Monte Carlo simulation of self-assembled polymer chains with inter-chain attractions** XINJIANG LÜ, JAMES KINDT, Emory University — We have used Monte Carlo simulations to study the phase behavior of self-assembled semiflexible chain polymers with inter-chain attractions. Approximate phase diagrams are obtained with varied physical parameters, such as the chain flexibility, intra- and inter-chain bonding energies. The attraction induced phase separation results in an equilibrium between a bundle and isotropic short chains. The chain length distribution of the phase separated system, as well as the bundle's shape and aspect ratio are presented and discussed. Simulation results are analyzed and compared with related experimental and theoretical work. We also present some other interesting results of observed toroids and branched bundles.

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