Abstract Submitted
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Minimal energy packings of weakly semiflexible polymers: Application to targeted self-assembly of nanostructures[1] JARED HARWAYNE-GIDANSKY, Electrical Engineering and Integrated Graduate Program in Physical and Engineering Biology, Yale University, ROBERT S. HOY, COREY S. O'HERN, Mechanical Engineering & Materials Science, and Physics, Yale University — Using exact enumeration, we characterize how structure, mechanical and thermodynamic stability of minimal energy packings of short "sticky tangent sphere" (SHS) polymer chains vary with angular interaction strength k_b and equilibrium bond angle θ_0. While flexible SHS polymers possess highly degenerate ground states (i. e. many differently ordered "macrostates" [1]), angular interactions dramatically break this degeneracy. The macrostate associated with the ground state semiflexible packing changes as k_b and θ_0 are varied. Further degeneracy breaking arises from angular interactions' influence on packing size, asymmetry, and vibrational entropy. The strength of these effects increases with chain length N. Our exact analysis provides design principles for self-assembly of polymers into a variety of structures that can be tuned by varying N, k_b and θ_0.

[1] R. S. Hoy and C. S. O'Hern, Phys. Rev. Lett. **105**, 068001 (2010).

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