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Linear aggregation and liquid-crystalline order: comparison of Monte Carlo simulation and analytic theory TATIANA KURIABOVA, University of Colorado, M.D. BETTERTON, MATTHEW A. GLASER, University of Colorado at Boulder — Many soft-matter and biophysical systems are composed of monomers that reversibly assemble into rod-like aggregates. The aggregates can then order into liquid-crystal phases if the density is high enough, and liquid-crystal ordering promotes increased growth of aggregates. Systems that display coupled aggregation and liquid-crystal ordering include wormlike micelles, chromonic liquid crystals, DNA and RNA, and protein polymers and fibrils. Coarse-grained molecular models that capture key features of coupled aggregation and liquid-crystal ordering common to many different systems are lacking; in particular, the roles of monomer aspect ratio and aggregate flexibility are not well understood. We study a system of sticky cylinders that interact primarily by hard-core interactions but can stack and bind end to end. We use Monte Carlo simulations and analytic theory. We present results for several different cylinder aspect ratios and a range of end-to-end binding energies. The phase diagrams are qualitatively similar to those of chromonic liquid crystals, with an isotropic-nematic-columnar triple point. Our analytic theory shows improvement compared to previous theory in quantitatively predicting the I–N transition for relatively stiff aggregates, but requires a better treatment of aggregate flexibility.

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