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Phase Behavior of Disk-Coil Macromolecules YONGJOO KIM, EDWARD HA, ALFREDO ALEXANDER-KATZ, MIT — We explore the self-assembly of disk-coil macromolecules using Monte Carlo simulations in the NPT ensemble. Our study focuses on the role that coil length compared to the size of the disk has on the phase behavior of the system as well as the effect of stacking interactions between the disks. As a function of temperature T, we find a disordered phase at high T and lamellar, perforated lamellar, and cylinder phases at intermediate T. If we further lower the temperature, the disk-rich regions spontaneously order, and we find ordered lamellar, ordered perforated lamellar, and ordered cylinder phases depending on the strength of the stacking interactions. The appearance of any of these phases is, however, strongly dependent on the length of the coil. In addition to constructing a comprehensive phase diagram, we further analyze the correlations in the system, as well as the director vector field of the disks, and use it to construct an order parameter. We show that the latter changes drastically at the ordering transition points. We find that the ordered cylinder phase has a high degree of parallel packing. Our results are important to understand the self-assembly of supramolecular structures of disk-coil amphiphiles that are ubiquitous in nature, such as the chlorophyll molecule.

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