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Self-Assembly of End-to-Tail Associating Liquid Crystalline Polymers MICHAEL RICHTER, ELENA DORMIDONTOVA, Polymer Program, Institute of Materials Science and Physics Department, University of Connecticut, Storrs, Connecticut 06269, United States — Self-assembly plays a central role in obtaining new responsive nanomaterials. The variety of the chemical nature of the building blocks and associating units creates a large spectrum of materials with controllable properties. To understand the self-assembly of a class of such materials we study a model rigid cylinders with attractive semi-spherical end-caps (spherocylinders). Using Monte Carlo simulations we study self-assembly of spherocylinders as a function of associating energy and spherocylinder concentration. Depending on the orientational specificity of association very different phase behaviors are observed. Systems with high orientational specificity of association form preferentially linear-shaped aggregates and are capable of achieving nematic order at sufficiently high concentration and association energy. Spherocylinders with low orientational specificity are capable of multiple associations between the end-caps, which results in network or scaffold-like structure formation depending on spherocylinder concentration. The corresponding phase behavior will be discussed.

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