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Rod-Coil Block Copolymer Simulation With SCFT LEE TRASK, ERIC COCHRAN, Iowa State University — Theoretical and experimental investigations of rod-coil block copolymer systems have made leaps forward recently. Fully 3D computer simulations of rod-coil diblock copolymer systems using self-consistent field theory (SCFT) have become feasible due to advances in theory and computer resources, while a number of experimental papers have illustrated a wide array of phases. These simulations include the use of all spatial and orientational degrees of freedom along with a Maier-Saupe interaction to describe the rod-rod alignment interactions. However, these 3D simulations have not been compared to experimental data. Simulations of moderately segregated poly(alkoxyphenylenevinylene-*b*-isoprene) (PPV-*b*-PI) are performed for a range of characteristic parameters linked to these systems. For different Flory-Huggins parameters, compositions, Maier-Saupe parameters, and geometric asymmetries, phase diagrams are constructed and compared with the phase diagrams previously reported in the literature. Along with phase space information, the domain space scaling relationship of the lamellar phase as a function of molecular weight is compared.

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