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Regioregularity-

Driven Phase Transition of Poly(3-hexylthiophene)-Based Block Copolymers JIN-SEONG KIM, YONGJOO KIM, HYUN-JEONG KIM, HYEONG JUN KIM, HYUNSEUNG YANG, YEON SIK JUNG, KAIST, GILA E. STEIN, University of Tennessee, Knoxville, BUMJOON J. KIM, KAIST — Conjugated polymerbased block copolymers (BCPs) offer great potential to provide beneficial nanostructures for efficient organic opto-electronics. However, their complicated self-assembly behavior, attributed to the strong crystallization of the conjugated blocks, is still not well understood due to the lack of a model BCP system. Herein, we develop a series of novel conjugated BCPs, poly(3-hexylthiophene)-block-poly(2-vinylpyridine) (P3HT-b-P2VP), in which the regionegularity (RR) of the P3HT block was varied from 95 to 73%. The tunable RR content allows for precise regulation of P3HT crystallization with minimal influence on the microphase-separation force between two blocks. When RR is high (95 or 85%), the structure is characterized by P3HT nanofibrils in an amorphous matrix. In contrast, as RR decreases to 78 and 73%, P3HT crystallization is suppressed, self-assembly is dominated by the enthalpic interaction, and thermal annealing drives the formation of well-ordered lamellar or cylindrical phases. This morphological behavior is consistent with a Monte Carlo simulation based on our coarse-grained model. Significantly, this novel class of RRcontrolled BCPs provides a simple method to tune phase behavior for a variety of applications in nanostructured organic electronics.

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