

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Simple Coarse-grained modeling of regioregularity controlled P3HT molecules YONGJOO KIM, HYEONG JUN KIM, JIN-SEONG KIM, YEON SIK JUNG, BUMJOON J. KIM, Korea Adv Inst of Sci & Tech — Conjugate polymers have been evaluated as the active component in organic electronics due to their great potential in the mass production of large area, light-weight and flexible electronic devices by cost-effective solution processing. Among them, poly(3-hexylthiophene) (P3HT) represents most widely investigated model system due to its high performances in various organic electronics. Among the various factors that affects the intrinsic properties of P3HTs, regio-chemical control over head-to-tail (HT) coupling between thiophene rings, defined by regioregularity (RR), has been considered most critical factor for the primary crystalline structure and resulting optoelectronic properties. Alkyl side chains in irregularly substituted head-to-head (HH) linkages causes a sterically driven twist of thiophene rings, resulting in a loss of conjugation and crystallinity. In this study, we suggest highly efficient coarse-grained model of RR controlled P3HT to study thermodynamical properties. We found that our P3HT model successfully predicts crystalline temperature as a function of RR and phase diagram of solution assembled RR controlled P3HT. We believe that our model can be efficiently used for designing various organic electronic devices based on RR controlled P3HT.

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Date submitted: 13 Apr 2017

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