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Predicting nematic coupling constants of semiflexible polymers from MD simulations WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State University — The nematic phase is important for many semiflexible polymers. For example, semiflexible polymers with nematic phase can be directly used in many applications, including displays and high strength fibers. The existence of nematic phases also enables better processing of functional semiflexible polymers including conducting conjugated polymers. The nematic coupling constant α, together with the chain stiffness κ, governs chain alignment and the isotropic-to-nematic (IN) transition temperature T_{IN} for semiflexible polymers. For many semiflexible chains, crystallization or thermal degradation can preclude the IN transition, so that T_{IN} cannot be used to estimate α. We combine self-consistent field theory (SCFT) with atomistic molecular dynamics (MD) simulations of semiflexible chains under external tension in the isotropic phase to estimate the nematic coupling constant α. Using our mean-field model, we can obtain the variational free energy of a given polymer, from which the IN transition temperature T_{IN} can be determined. We apply our method to estimate α and T_{IN} of a commonly studied conjugated polymer, poly(3-hexylthiophene) (P3HT). Using the estimated T_{IN}, we predict P3HT is nematic after melting from crystal.

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