Demixing by a Nematic Mean Field: Coarse-Grained Simulations of Liquid Crystalline Polymers

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In this work we have used a coarse-grained formalism to study the phase behavior of semi-flexible nematic polymers in pure melts and mixtures.

- We have explored the conditions that lead to macrophase separation in mixtures of stiff and flexible polymers mediated by the orientational interaction in otherwise identical polymers.
- We have found that in macroscopic samples the kinetics of phase separation will lead to formation of non-equilibrium morphologies where nematic domains form a percolating network that spans the whole sample.
- The latter structures are of interest for the development of photovoltaic organic devices.
- The formalism used in this work should therefore provide a strategy for systematic coarsening from atomistic simulations to coarse-grained representations and vice versa.

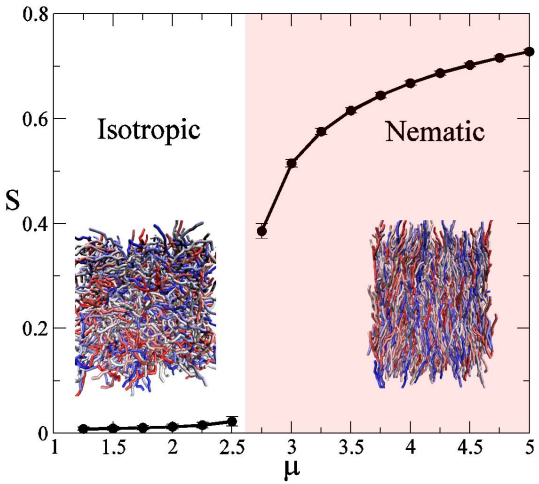

Figure 1. Global order parameter, S, as a function of the orientational coupling m, obtained by Monte Carlo simulations (symbols). Polymer chains are composed of N = 8 segments, and k = 3.5. Lines are only a guide to the eye. Insets are instantaneous polymer configurations in the isotropic and nematic phases, different chain colors are used to facilitate visualization.

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