

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Simulations of liquid crystalline phases of semiflexible polymer melts and blends KIRAN KHANAL, JUTTA LUETTNER-STRATHMANN, Departments of Chemistry and Physics, The University of Akron — We perform Monte Carlo simulations of a bond-fluctuation model for polymers and introduce a bending energy so that polymer chains are flexible at high temperatures and rod like at low temperature. The phase diagram of polymer melts is determined in the temperature-density plane and the isotropic to nematic transition temperature is found to increase with increasing density. Single chain properties show that coupling between density and stiffness effects lead to nematic order. Blending with flexible chains leads to microphase separation and the formation of ordered domains of rods embedded in disordered regions.

Kiran Khanal
University of Akron

Date submitted: 09 Nov 2012

Electronic form version 1.4