Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

From gas-liquid to liquid crystalline phase behavior via anisotropic attraction: A computer simulation study in three and two dimensions REINHARD HENTSCHKE, Fachbereich Mathematik und Naturwissenschaften, Bergische Universitaet, 42097 Wuppertal, Germany, WEN-ZE OUYANG, National Microgravity Laboratory, Institute of Mechanics, Chinese Academy of Science, Bejing 100190, P. R. China — The partial phase behavior of a continuum molecular model for self-assembling semiflexible equilibrium polymers is studied via Monte Carlo and Molecular Dynamics simulation. We investigate the transfer from ordinary gas-liquid coexistence to the appearance of liquid crystallinity driven by excluded volume interaction between rod-like aggregates. The transfer between the two types of phase behavior is governed by a tunable anisotropic attractive interaction between monomer particles. The relation to dipolar fluid models, which are also known to form reversible chains, is discussed. In two dimensions, depending on the strength of the anisotropy, we find the formation of reversible networks as well as stiff rod-like aggregates. The phase transition observed in the presence of the network structures is compared to predictions of the Tlusty-Safran defect model.

Reinhard Hentschke
Bergische Universitaet, 42097 Wuppertal, Germany

Date submitted: 11 Nov 2009 Electronic form version 1.4