Contribution ID: **12** Type: **Invited Speaker / Conférencier invité**

WITHDRAWN Monte Carlo Field-Theoretic Simulations for Melts of Diblock Copolymer

Tuesday 17 June 2014 14:45 (30 minutes)

Monte Carlo field-theoretic simulations (MC-FTS) are performed on melts of symmetric diblock copolymer for polymerization indices extending down to experimentally relevant values. The simulations are performed with a fluctuating composition field and a pressure field that follows the saddle-point approximation. Our study focuses on the disordered-state structure function, S(k), and the order-disorder transition (ODT). Although short-wavelength fluctuations cause an ultraviolet (UV) divergence in three dimensions, this is readily compensated for with the use of an effective Flory-Huggins interaction parameter. The resulting S(k) matches the predictions of renormalized one-loop (ROL) calculations over the full range of parameters examined in our study, and agrees well with Fredrickson-Helfand (F-H) theory near the ODT. Consistent with the F-H theory, the ODT is discontinuous and the shift in the ODT follows the predicted scaling.

Author: Prof. MATSEN, Mark (University of Waterloo)

Presenter: Prof. MATSEN, Mark (University of Waterloo)

Session Classification: (T2-6) Biophysics/Soft Condensed Matter I: Polymers - DCMMP-DMBP / Biophysique et matière condensée molle 1: polymères - DPMCM-DPMB

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)