Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Fluctuations/Correlations in Symmetric Diblock Copolymers: Simulations and Theories JING ZONG, DELIAN YANG, QIANG (DAVID) WANG, Department of Chemical and Biological Engineering Colorado State University — Modeling symmetric diblock copolymers as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations, we have performed fast off-lattice Monte Carlo (FOMC) simulations1 in a canonical ensemble with variable box lengths to study the thermodynamic and structural properties of both the disordered and lamellar phases. Our FOMC results for the disordered phase are further compared, without any parameter-fitting, to those from the reference interaction site model (RISM) and the polymer reference interaction site model (PRISM) theories, as well as the Gaussian fluctuation theory, based on the same model system. Such direct comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers.

[1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

Jing Zong
Department of Chemical and Biological Engineering
Colorado State University

Date submitted: 12 Dec 2011 Electronic form version 1.4