Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Single-Chain in Mean-Fied simulations for Block Copolymer/Nanoparticle Composites FRANCOIS DETCHEVERRY, YIORYOS PAPAKONSTANTOPOULOS, HUIMAN KANG, PAUL NEALEY, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, 1415 Engineering Drive, Madison, WI 53706, KOSTAS DAOULAS, MARCUS MUELLER, Institut fur Theoretische Physik, Georg-August Universitat, 37077 Goettingen, Germany — Incorporating nanoparticles into self-assembling copolymers is a promising route towards creation of structures tailored at the nanometer scale and for design of new functional materials. However, predicting the behavior of nanoparticles dispersed in diblock copolymers remains a theoretical challenge. We have developed a single-chain in mean-field simulation technique that permits study of copolymer/nanoparticle composites in two limits, including hard and soft nanoparticles. The models proposed in this work are capable of describing the morphological changes induced by adding nanoparticles to block copolymers, and the distribution of nanoparticles in block copolymer thin films on patterned substrates.

Francois Detcheverry
Department of Chemical and Biological Engineering,
University of Wisconsin-Madison

Date submitted: 12 Dec 2006 Electronic form version 1.4