Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theory and Simulation Studies of Copolymer Functionalized Nanoparticles in Polymer Nanocomposites ARTHI JAYARAMAN, NITISH NAIR, AREZOU SEIFPOUR, PHILIP SPICER, University of Colorado at Boulder — Significant interest has grown around the ability to create polymer nanocomposites with controlled spatial arrangement of nanoparticles mediated by a polymer matrix. By functionalizing or grafting polymers on to nanoparticle surfaces and systematically tuning the composition, chemistry, molecular weight and grafting density of the functionalized polymers we can tailor the inter-particle interactions and precisely control the assembly/dispersion of the particles in the polymer matrix. While prior experimental and theoretical work in this area has mostly been on homopolymer grafted particles at high brush-like grafting densities, we study copolymer grafted nanoparticles at low grafting densities in a homopolymer matrix. Using an integrated approach involving Polymer Reference Interaction Site Model (PRISM) theory and Monte Carlo simulations we will present the effect of monomer sequence and molecular weight of the grafted copolymer, compatibility of the graft and matrix polymers, and nanoparticle size on the conformations of the grafted polymers, and the effective interactions between the grafted nanoparticles in the matrix.

Arthi Jayaraman
University of Colorado at Boulder

Date submitted: 19 Nov 2009 Electronic form version 1.4