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Nano-particle distribution in a polymer nano-composite PANAGIOTIS MANIADIS, Theoretical Division and CNLS, Los Alamos National Lab, IOANNIS N. TSIMPANOGIANNIS, Environmental Research Laboratory, National Center for Scientific Research "Demokritos", Greece, EDWARD M. KOBER, Institute of Multiscale Modeling and Simulations, Los Alamos National Lab, TURAB LOOKMAN, Theoretical Division, Los Alamos National Lab — We use the hybrid particle-Self Consistent Field calculation (hybrid particle-SCF) to study the distribution of particles in a multi-block copolymer nano-composite. Using the static approach, we first find the effective interaction potential between the nano-particles and the polymer. The interaction has an entropic and an enthalpic component. The dynamical simulation confirms that the distribution of particles has a maximum at the minima of the interaction potential. We also study the situation where the nano-particles are distributed in a blend of AB diblock and A homopolymer. In this case, for large homopolymer concentration (larger than 20%), an interface is created between components that are identical, but they come from different types of polymer chains (i.e. the AB diblock or the A homopolymer). We find that the interaction potential has a minimum in this A/A interface which is of pure entropic origin. Furthermore the dynamical simulation reveals that the distribution of nano-particles has a maximum in the area around this interface.

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