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Single Chain Mean Field Theory (SCMF) in Polymer Nanocomposites SUDEEPTO SEN, SANAT KUMAR, Columbia University, IGAL SZLEIFER, Purdue University — Recent experimental work in our group has shown that grafting the surface of inorganic nanoparticles with polymer brushes improves the dispersion of the particles in a polymer matrix. Since improved dispersion is critical to the enhancement in material properties of the resultant nanocomposite, we are motivated to study the thermodynamics of the interface structure in the polymer particle system since the interface itself is a major determinant of nanocomposite properties. We will present the results from recent and ongoing SCMF studies on a model polymer nanocomposite system with grafted particles and explore the thermodynamics of the particle/chain miscibility region along with explicit knowledge of the polymer chain structures (both matrix and grafted). Dependence on various parameters such as the molecular weights of the grafted and matrix chains respectively, the density of the grafted chains and the particle size will also be explored.

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