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Statistical Mechanical Theory of Effective Interactions, Structure and Phase Behavior of Polymer Nanocomposites LISA HALL, K.S. SCHWEIZER, University of Illinois at Urbana-Champaign — Microscopic polymer liquid state theory has been recently developed and extensively applied for the structure, thermodynamics and miscibility of model polymer nanocomposites composed of hard spherical fillers and flexible polymer chains [1]. The complex and often subtle interplay of coupled entropic (translational and packing) and enthalpic (interfacial cohesion) effects results in rich structural and phase behavior. New computational studies have established in detail the role of polymer degree of polymerization on the equilibrium behavior. The theory has been generalized to treat the consequences of soft intermolecular repulsions and van der Waals like attractions between all mixture species. In addition, nonspherical fillers of variable shape and effective dimensionality have been studied including rod, disk and compact molecule-like shapes. Both repulsive force softness and anisotropic filler shape affect the entropic and enthalpic aspects of the problem and can significantly modify their consequences on structure and phase behavior.

[1] J.B.Hooper and K.S.Schweizer, *Macromolecules* 38, 8858 (2005); 39, 5133 (2006).

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