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Many Body Effects on Particle Diffusion in Polymer Nanocomposites ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — Recent statistical mechanical theories of nanoparticle motion in polymer melts and networks have focused on the dilute particle limit. By combining PRISM theory predictions for microscopic structural correlations, and a new formulation of self-consistent dynamical mode coupling theory, we extend dilute theories to finite filler loading. As a minimalist model, the polymer dynamics are first assumed to be unperturbed by the presence of the nanoparticles. The long time particle diffusivity in unentangled and entangled melts is determined as a function of polymer tube diameter and radius of gyration, nanoparticle diameter, and polymer-filler attraction strength under both constant volume and constant pressure situations. The influence of nanocomposite statistical structure (depletion, steric stabilization, bridging) on dynamics is also investigated. Using recent theoretical developments for predicting tube diameters in nanocomposites, the consequences of filler-induced tube dilation on nanoparticle motion is established. In entangled melts, increasing filler loading first modestly speeds up diffusion, and then dramatically when the inter-filler separation becomes smaller than the tube diameter. At very high loadings, a filler glass transition is generically predicted.

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