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A Theoretically Informed Model for the Rheology of Entangled Block Copolymer Nanocomposites YONGRUI SU, The University of Chicago, ABELARDO RAMIREZ-HERNANDEZ, The University of Chicago and Argonne National Laboratory, BRANDON PETERS, The University of Chicago, JUAN J. DE PABLO, The University of Chicago and Argonne National Laboratory — The addition of nanoparticles to block copolymer systems has been shown to have important effects on their equilibrium structure and properties. Less is known about the non-equilibrium behavior of block polymer nanocomposites. A new particle-based, theoretically informed coarse-grained model for multicomponent nanocomposites is proposed to examine the effects of nanoparticles on the rheology of entangled block copolymer melts. Entanglements are treated at the two-molecule level, through slip-springs that couple the dynamics of neighboring pairs of chains. The inclusion of slip-springs changes the polymer dynamics from unentangled to entangled. The nanoparticles are functionalized with short polymer chains that can entangle with the copolymers. We study the nonlinear rheology of the resulting nanocomposites under shear flow with a dissipative particle dynamics (DPD) thermostat.

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