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Multi-Scale Polymer Conformations Between Confining Nanoparticles ERIC BAILEY, ROBERT A. RIGGLEMAN, KAREN I. WINEY, Univ of Pennsylvania — The addition of nanoparticles (NPs) to a polymer matrix is known to significantly enhance the mechanical and functional properties of the polymer. Despite recent research efforts, several structural and dynamic properties remain mechanistically and comprehensively unknown. This is especially true in the confined regime, when the interparticle distance (ID) is on the order of the size of the polymer chain (2Rg). Here, coarse-grained molecular dynamics simulations are used to systematically study the effect of ID on multi-scale polymer conformations as a function of ID and chain length (spanning unentangled and entangled chains). A monolayer of NPs are hexagonally packed and placed within bulk polymer, revealing the length scale and magnitude of perturbations caused by two or more confining NPs. When ID/2Rg>1, chains are flattened within Rg of the NP surface and bulk conformations are retained even between NPs. This is consistent with extrapolations from previous simulations using a single isolated particle. For ID/2Rg<1, preliminary results suggest that the perturbed chain profiles interact unexpectedly and chain-scale conformations may not be appropriate to describe chain distortions. These conformational changes and perturbations are expected to influence dynamic properties.

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