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Structure and dynamics of solvent-free polymer grafted nanoparticles: A computational study ALEXANDROS CHREMOS, ATHANASSIOS PANAGIOTOPOULOS, Chemical and Biological Engineering, Princeton University
— The structure and dynamics of solvent-free polymer-grafted nanoparticles have been investigated using molecular dynamics simulations. A basic coarse-grained model was used, where the nanoparticle is represented as a single smooth particle with bead- spring polymer chains attached to it. Motivated by the recent advances in nanoparticle ionic materials and nanoparticle organic hybrid materials, we use our model to explore the behavior of these systems over a wide range of parameters and gain insights of their structure and transport properties. In particular, we find that the chain length variation can change the softness of the nanoparticles, so for short chains the system exhibits rich structural characteristics while for long chains display (dilute) liquid-like characteristics. Additionally, we find that by increasing the softness of the particles the structural relaxation of the system becomes less sensitive to temperature variation, indicating a change from the hard-spheres to soft particles. The results confirm the experimental observations that changing the chain length the system can display behavior that spans from glasses to liquids.

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