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Molecular Dynamics Simulations on the Thermal and Mechanical Properties of Blend of Polymer and Polymer Grafted Nanoparticles
SANAT KUMAR, DONG MENG, Department of Chemical Engineering, Columbia University, GARY GREEST, Sandia National Laboratories — Grafting polymers onto the surface of NPs has become one of the most effective approaches to integrate NPs into polymer melts. It then becomes crucial to be able to understand how the presence of grafted chains affects the effective interactions between NPs as well as the mechanical properties of the resulting composites. Using molecular dynamics simulations we first measure the potential of mean force between grafted NPs from two-particle simulations. Simulations of systems containing many grafted NPs are then performed to determine the phase behavior and structure of grafted NPs in explicit polymer matrices. Finally, we cool the nanocomposites to temperatures below their glass transition and stress the systems to investigate how the presence of grafted NPs changes their mechanical properties.

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