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Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix NITISH NAIR, ARTHI JAYARAMAN, University of Colorado at Boulder — Functionalizing nanoparticles with small ligands or polymers is an effective way to tune the interfacial interactions between nanoparticles and in turn their spatial organization in a solvent or polymer matrix. We integrate Polymer Reference Interaction Site Model (PRISM) theory and Monte Carlo (MC) simulations to study copolymer-functionalized nanoparticles embedded in a polymer melt. While PRISM theory can be applied to dense systems with minimal computational effort, it involves approximations, e.g. the use of ideal conformations for the grafted and free polymers. On the other hand, MC simulations of polymer melts are computationally intensive but devoid of the approximations of PRISM. Therefore, we combine the advantages of each method by presenting a self-consistent PRISM-MC approach which gives us theoretical results that are more accurate than pure PRISM theory at packing fractions that are hard to access with pure MC simulations. Using this self-consistent PRISM-MC approach, we have studied the effect of packing fraction and the sequence of the grafted polymers on the potential of mean force between two copolymer-grafted nanoparticles in a homopolymer matrix.

Nitish Nair
University of Colorado at Boulder

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