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Meso-scale Modeling of Self-assembly of Polymer-Grafted Nanoparticles[1] DERRICK MANCINI, Illinois Inst of Tech, SANKET DESHMUKH, SUBRAMANIAN SANKARANARAYANAN, Argonne National Laboratory — We develop meso-scale models to explore the self-assembly behavior of polymer-grafted nanoparticles. Specifically, we study nanoparticles with grafts of the thermo-sensitive polymer poly(N-isopropylacrylamide) (PNIPAM), which undergoes a coil-to-globule transition across the LCST at around 305 K. The atomic-scale mechanism of the coil-to-globule transition of polymers grafted nanoparticles and their interactions (agglomeration, assembly behavior) with other particles that are in its vicinity is poorly understood, yet knowledge about these interactions would enable designing novel self-assembled materials with well-defined structural and dynamical properties. Additionally, the effects of chemical nature, geometry, and morphology of the nanoparticle surface on the conformational transition of thermo-sensitive polymers is also unknown. We report on 1) development of all-atom models of polymer-grafted nanoparticles to conduct MD simulations at atomic-levels and 2) perform mesoscopic scaling of the conformational dynamics resulting from the atomistic simulations with the aid of coarse-grained or meso-scale models of PNIPAM and its composites. Coarse-grained simulations allow modeling of larger assemblies of polymer-grafted nanoparticles over longer time scales.

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