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Multi-Million-Atom Molecular Dynamics Simulations of Polymer Nanoparticle Composites using Explicit Solvent Treatment SANKET DESHMUKH, Argonne National Laboratory, GANESH KAMATH, University of Missouri-Columbia, DERRICK MANCINI, SUBRAMANIAN SANKARANARAYANAN, Argonne National Laboratory — Poly(N-isopropylacrylamide) (PNIPAM) is a thermosensitive polymer that is well-known for its lower critical solution temperature (LCST) around 305K. Below the LCST, PNIPAM is soluble in water, and above this temperature, polymer chains collapse and transform into a globule-state. Our simulations of systems consisting of single polymer chains in presence of explicit water molecules ($\sim$ 50 K atoms) predicted the LCST of PNIPAM close to the observed experimental value of $\sim$ 305 K. This study also suggested the importance of using an explicit water model in studying the coil-to-globule transition in thermo-sensitive polymers. In the current studies, we are carrying out MD simulations of composites of PNIPAM inorganic nanoparticles in the aqueous solution using an explicit solvent treatment. We study the effect of grafting density on the coil-to-globule transition of the PNIPAM brushes. We graft PNIPAM polymer chains consisting of 60 monomer units onto a gold nanoparticle with varying grafting densities. Studied system consisted of $\sim$3 million atoms. All the simulations were carried out below (275K) and above (325K) the LCST of PNIPAM. Simulation trajectories are analyzed for structural and dynamical properties. In particular, we look at the morphology of the uncollapsed and collapsed structures, and relate this to observation in scattering measurements. Future work will expand this approach to studying the dynamics of agglomeration of such brush structures to form self-assembled nanocomposites.

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