Understanding phase behavior and mechanical properties of polymer grafted nanoparticles

Fernando Escobedo

Polymer grafted Nanoparticles in homopolymer solvents or PGNs have become increasingly popular in mechanical, optical and electrical applications due to their ability to improve the properties of the host matrix. Dispersion of PGNs in host matrix is necessary to achieve the desired properties in these hybrid nanomaterials. These systems transition into mixed (dispersed) and demixed (phase separated) state depending on the molecular design and interactions between the grafted polymer and host matrix, with a marked difference in properties between these two states. To establish whether a PGN system will undergo a mixed to demixed transition one needs to calculate the free energy difference between the dispersed and aggregated states. We thus aim to use mesoscale modelling to calculate the free energy difference associated with the mixed to demixed transition in PGN and homopolymer system. To this end, we will implement umbrella sampling calculations that use a biasing field, based on a local-composition-based order parameter, to sample configurations continuously from the mixed to the demixed regions of the phase space to obtain the underlying free energy landscape.

We will also study the viscoelastic behavior of PGN systems with attractive solvent and grafted chain interactions. These dispersed systems show a richer viscoelastic behavior characterized by higher viscosity and storage and loss moduli on increasing loading of nanoparticles. We aim to elucidate how modifications of the interaction parameters (to represent specific chemistries), and PGN characteristics affect the physical character of the resulting composites which can range from waxes and gels at high loading to low viscosity fluids at low loading. This work is complementary to some of the experimental work in Prof. Archer's Lab.