Talk Title:
Nanoparticles in solution – interactions and asymmetries through molecular simulation

Abstract:
Nanoparticles and nanoscience are increasingly critical to a host of energy and technology applications. However, making use of nanoparticles often requires coating them to improve their usability. For instance, nanoparticles in solution are often stabilized with coatings to prevent aggregation. I will discuss how these coatings affect the forces between nanoparticles and present recent molecular dynamics simulation results showing that small spherical nanoparticles produce highly asymmetric coating arrangements, when coated with commonly-used simple polymer chains. These coatings are not symmetric even when one would think they should be. I will discuss the geometric properties which dictate the coating shape and their implications. When particles are placed at the solvent surface, the asymmetric coatings are amplified and oriented by the surface. Particle shape and its responsive behavior is seen to strongly influence interactions. Implications and examples of controlled self-assembly will be presented.