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DNA Directed Nanoparticle Assemblies[1]

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While DNA is mostly noted for carrying genetic information, a single strand of DNA is simply a polymer with chemically specific recognition. As a result, DNA is an interesting polymer to consider for the development of new materials. In particular, attaching single strands of DNA to nanoparticles offers the possibility to encode highly specific bonding between nanoparticles to create engineered building blocks, or "functionalized atoms." These core units are an ideal candidate for the development of network-based, nanostructured materials. In this talk, we present results from computer simulations of a coarse-grained model examining several choices and DNA functionalization, and show how these design choices can affect dynamics, phase behavior, and the formation of crystal structures. We first discuss nanoparticles functionalized by four single DNA strands. These units give rise to a material with a hierarchy of interpenetrating networked structure and four thermodynamically distinct amorphous phases, unlike any naturally occurring pure material. On the other hand, the mechanism for the formation of the amorphous phases offers insight into anomalous networked liquids like water and silica. We also consider how varying the number of functionalizing DNA strands alters both the number and shape of these phase transitions. The formation of very low density crystals of nanoparticles tethered by DNA has recently been achieved experimentally, but the factors controlling crystal formation are still not well understood. Therefore, we also discuss the results of nanoparticles uniformly coated with DNA, similar to experimental systems. We show how the DNA strand length and stiffness affects the competition between energy and entropy that controls crystal formation.

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