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Computer Simulation of Ligated Nanoparticle Assembly from Solution FLINT PIERCE, AMIT CHAKRABARTI, CHRIS SORENSEN, Kansas State University — Nanoparticles are becoming increasingly important for the design of novel materials in a wide range of new applications. Ligation of these particles by chemical species provides a means to stabilize them into useful assemblies. It is essential to have a clear physical picture of the way these particles interact. To this end, we are investigating systems of metal nanoparticles ligated with alkyl chains. Our approach is three-fold. First, we are simulating (Monte Carlo) systems of ligated nanoparticles, including all chain/particle interactions in order to develop a model potential. Second, we are simulating (molecular dynamics) systems of these particles interacting via this model potential, varying the alkyl chain length, solvent, core material, and particle volume fraction. Finally, for comparison we are simulating these systems using theoretically derived potentials found in the literature. Initial results indicate a range of morphologies, from fractal aggregates to crystallites, depending on the temperature and potentials involved. Our goal is to provide a guide to researchers in choosing materials and assembly conditions that will lead to desired assembly properties.

Flint Pierce
Kansas State University

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