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Self-Assembly of Ligated Gold Nanoparticles[1] A. CHAKRABARTI, S.J. KHAN, C.M. SORENSEN, Kansas State University — We study assembly of ligated gold nanoparticles by both phenomenological modeling and computer simulations for various ligand chain lengths. First, we develop an effective nanoparticle-nanoparticle pair potential by treating the ligands as flexible polymer chains. Besides van der Waals interactions, we incorporate both free-energy of mixing and elastic contributions from compression of the ligands in our effective pair potentials. Next, we use the calculated pair potentials as input to Brownian Dynamics simulations for studying nucleation and growth of nanoparticle superlattice formation in three dimensions.

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