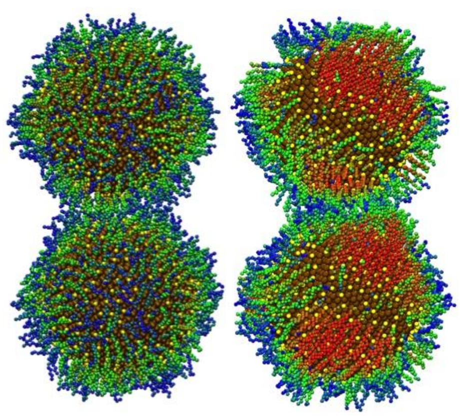
Influence of microstructure and environment on nanoparticle membrane and superlattice mechanical properties

K. Michael Salerno
Center for Integrated Nanotechnologies
Sandia National Laboratories
Albuquerque, NM

Assembly of nanoparticles (NPs) offers a means to tailor materials, incorporating unique nanoscale behavior with controllable, responsive mechanical properties. Organic NP ligand coatings provide a way to drive assembly and control assembly properties. Atomistic molecular-dynamics simulations of alkanethiol-coated gold nanoparticles are used to examine how coating chemistry, temperature, and assembly history affect the properties of two-dimensional NP membranes and three-dimensional NP superlattices. Specifically, NPs coated with dodecanethiol and octadecanethiol ligands with COOH or CH_3 end groups are assembled into two-dimensional membranes at liquid/vapor interface. Orientational order in the NP coating indicates that ligands strongly bundle and orient. Replacing terminating methyl groups with hydrogen-bond forming carboxyl groups more than doubles the membrane Young's modulus from 1.7 to 3.6 GPa. We observe that the liquid/vapor interface asymmetry leads to a measurable and persistent stress asymmetry in membranes. Simulations also show that within three-dimensional superlattices large deviatoric stresses can lead to failure of the ligand-core bond, and experiments show that core sintering can occur, creating novel gold structures. Molecular dynamics time and length-scale limitations have recently prompted us to model nanoscale systems using coarse-grained methods, which I will briefly discuss.



Dodecanethiol-coated gold NPs (D=6nm) show dramatically different ligand ordering (carbon colored according to orientation order parameter) at 400K (left) and 300K (right).