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

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Assembly of nanoparticles (NPs) offers a means to tailor materials, incorporating unique nanoscale electro-optical behavior with controllable, responsive mechanical properties. Encoding NPs with organic ligands provides a way to simultaneously 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 nanoparticle membranes and three-dimensional nanoparticle superlattices. Specifically, NPs were coated with dodecanethiol and octadecanethiol ligands with COOH or CH₃ end groups and assembled into two-dimensional membranes at water vapor interface. Capping ligands with hydrogen-bond forming carboxyl groups rather than methyl groups more than doubles the membrane Young's modulus from 1.5 to 3.6 GPa. The orientational order of the coating oligomers indicates that ligands strongly bundle and orient within the membrane. This effect inhibits ligand interdigitation, decreasing stiffness. Ligand structure is also highly temperature dependent, causing membranes to lose mechanical stability at about 400K. We observe that the interface asymmetry leads to a measurable stress asymmetry. Due to buckling, stresses in 2D membranes are typically quite small, however 3D superlattices can reversibly reach pressures of 8 GPa. Simulations show that at these pressures the ligand-core bond can be an important failure point, and experiments show that core sintering occurs at high pressure, creating novel 3D and quasi-2D structures.

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