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Structure and Stability of Self-Assembling Nanoparticle Dispersions[1]

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Nanoparticles have attracted much attention because of their unusual electronic and optical properties, e.g., photoluminescence, which are intermediate between those of bulk and molecular materials. Applications to thin-film photovoltaic devices are facilitated by self-assembly of nanoparticles into a crystalline array (superlattice). By coating nanoparticles with ligand brushes, bulk dispersions can be sterically stabilized against aggregation induced by van der Waals forces. Creating equilibrium superlattices in the laboratory, however, remains a practical challenge. To investigate the dependence of superlattice stability on interparticle forces, we perform molecular dynamics and Monte Carlo simulations to model bulk dispersions of silicon and silver nanoparticles, governed by effective pair potentials that combine short-range steric and long-range van der Waals forces. From particle configurations, we compute radial distribution functions and static structure factors to explore equilibrium structure and phase stability. By varying ligand length and bulk density, we characterize the tendency of nanoparticles to self-assemble into ordered arrays or amorphous clusters. Our results may guide the design of future experiments and fabrication of superlattices.

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