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Control of DNA-Functionalized Nanoparticle Assembly

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Directed crystallization of a large variety of nanoparticles, including proteins, via DNA hybridization kinetics has led to unique materials with a broad range of crystal symmetries. The nanoparticles are functionalized with DNA chains that link neighboring functionalized units. The shape of the nanoparticle, the DNA length, the sequence of the hybridizing DNA linker and the grafting density determine the crystal symmetries and lattice spacing. By carefully selecting these parameters one can, in principle, achieve all the symmetries found for both atomic and colloidal crystals of asymmetric shapes as well as new symmetries, and drive transitions between them. A scale-accurate coarse-grained model with explicit DNA chains provides the design parameters, including degree of hybridization, to achieve specific crystal structures. The model also provides surface energy values to determine the shape of defect-free single crystals with macroscopic anisotropic properties, as well as the parameters to develop colloidal models that reproduce both the shape of single crystals and their growth kinetics.