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Multi-scale modeling for the self-assembly of DNA-functionalized nanoparticle into supperlattice and Wulff polydedra[1] TING LI, EVELYN AUYEUNG, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University, NORTHWESTERN UNIVERSITY TEAM — Since 1996, DNA hybridization has proven robust for programmable self-assembly of nanoparticles (NPs). Recently, we showed that through a "slow cooling" method, DNA functionalized nanospheres or so-called "programmable atom equivalents" can assemble into crystals with a specific and uniform habit. Here we perform molecular dynamics simulations on multi-scale models to study and predict the corresponding shapes. Firstly, we use a scale-accurate coarse-grained model with explicit DNA chains to estimate surface energy ratios for different surface orientations, and predict the corresponding Wulff polyhedra based on these values. Secondly, we use a colloidal model in which each DNA coated nanosphere is represented by a single bead to simulate the growth dynamics of the crystals. By this method, we confirm the shape for the body-centered-cubic system to be a (110)-enclosed rhombic dodecahedron. But the face-centered-cubic system does not show any uniform shape yet except triangular features with (111) and (100) facets due to crystallographic defects including twinning and stacking faults. These simulated crystal shapes agrees very well with experiments.

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