

Abstract Submitted
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DNA-programmable Nanoparticle Self-Assembly and Crystallization via Multi-Scale Modelling & Simulation¹ TING LI, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, NORTHWESTERN UNIVERSITY TEAM — In the past decades, DNA hybridization has proven promising to rationally guide nanoparticles to assemble into 1D, 2D and 3D structures, lattices and recently, faceted single crystals. In this sense, a gold nanoparticle coated by a dense shell of DNA behaves as a “programmable atom equivalent.” Using a scale-accurate coarse-grained model with explicit DNA chains, we identify that the key ingredient for achieving successful 3D crystallization is in the kinetics of DNA hybridization. We predict phase diagrams and propose suitable DNA linker sequences for optimal assembly. We determine the equilibrium shape of single crystals by computing surface energies. Surface energy fluctuations are further estimated for different surface orientations, and are shown to be critical in determining the equilibrium shape of a crystal. In addition, we apply a colloidal model with implicit DNA chains to study the kinetics of crystallization into faceted single crystals.

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