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Self-Assembly of Octopus Nanoparticles into Pre-Programmed Finite Clusters¹ JONATHAN HALVER-SON, ALEXEI TKACHENKO, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973 — The precise control of the spatial arrangement of nanoparticles (NP) is often required to take full advantage of their novel optical and electronic properties. NPs have been shown to self-assemble into crystalline structures using either patchy surface regions or complementary DNA strands to direct the assembly. Due to a lack of specificity of the interactions these methods lead to only a limited number of structures. An emerging approach is to bind ssDNA at specific sites on the particle surface making so-called octopus NPs. Using octopus NPs we investigate the inverse problem of the self-assembly of finite clusters. That is, for a given target cluster (e.g., arranging the NPs on the vertices of a dodecahedron) what are the minimum number of complementary DNA strands needed for the robust self-assembly of the cluster from an initially homogeneous NP solution? Based on the results of Brownian dynamics simulations we have compiled a set of design rules for various target clusters including cubes, pyramids, dodecahedrons and truncated icosahedrons. Our approach leads to control over the kinetic pathway and has demonstrated nearly perfect yield of the target.

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