K.L. Kohlstedt, M. Olvera de la Cruz and G.C. Schatz deduced the design rule for DNA-linker coated Au-Nanoprisms that is dependent on the ratio of two natural length scales of the nanostructure: the length of dsDNA spacer and the edge length of the prism. In the paper we use a novel coarse-grained model to track the short-range order of the prisms during the assembly of the superlattice and predicts the transition from 1D periodic arrays to 3D fcc arrangements. These phase transitions can be generalized for other polyhedra superlattices and will provide synthetic chemists a guide in the design of DNA coated polyhedra.

Unlike isotropic polyvalent assemblies, we find that the highly oriented chains of prisms lose orientational order in discrete steps during melting as the prisms in the arrays dissociate. We predict this multistage melting inhibits superlattice growth and is a direct consequence of the restriction in degrees of freedom from the face-to-face coordination of the multivalent prisms.

The complex behavior of the shape in nanostructure assemblies allows for novel applications especially in the area of plasmon coupling. Simple design rules for lattice structures are key toward developing a framework between nanostructure shape and the coordination of the assembly. Given the increasing complexity in the possible shapes of nanostructures and the specificity of DNA oligomers, we expect that design rules will become key in predicting the properties of the assembled structures.

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