Programmable Self-Assembly of Nanoplates into Bicontinuous Nanostructures

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Self-assembly is the process by which individual components arrange themselves into an ordered structure by changing shapes, components, and interactions. It has enabled us to construct a remarkable range of geometric forms at many length scales. Nevertheless, the potential of two-dimensional polygonal nanoplates to self-assemble into extended three-dimensional structures with compartments and corridors has remained unexplored. We show coarse-grained Monte Carlo simulations demonstrating self-assembly of hexagonal/triangular nanoplates via DNA-mediated complimentary interactions into facetted, sponge-like "bicontinuous polyhedra" (or infinite polyhedra) whose flat walls partition space into a pair of mutually interpenetrating labyrinths. Two bicontinuous polyhedra can be self-assembled: the regular (or Platonic) Petrie-Coxeter infinite polyhedron (denoted {6,4|4}) and the semi-regular Hart "gyrangle". The latter structure is chiral, with both left- and right-handed version. We show that the Petrie-Coxeter assembly is constructed from two complementary types of hexagonal nanoplates. Remarkably, we find that the 3D chiral Hart gyrangle can be assembled from one-component achiral triangular nanoplates decorated with regioselective complementary DNA interaction sites. In addition, Petrie-Coxeter and Hart assemblies are facetted versions of two of the simplest triply periodic minimal surfaces, namely Schwarz' Primitive and Schoen's Gyroid surfaces respectively, offering new routes to those bicontinuous nanostructures, which are widespread in synthetic and biological materials.

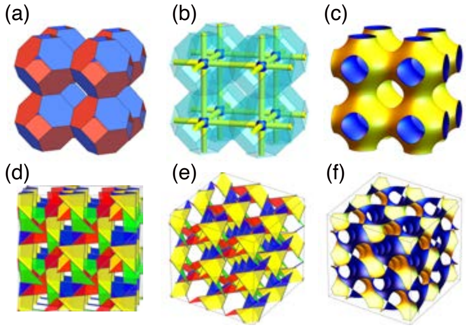

Figure 1 Infinite bicontinuous polyhedra. (a) {6,4|4} regular infinite polyhedron ($Im\bar{3}m$). (b) Jungle-gym labyrinth. (c) The Primitive surface. (d, e) Two views of a "gyrangle", another regular infinite polyhedron ($I4_132$). The gyrangle consists of four sets of parallel triangles. (f) The Gyroid surface ($Ia\bar{3}d$).

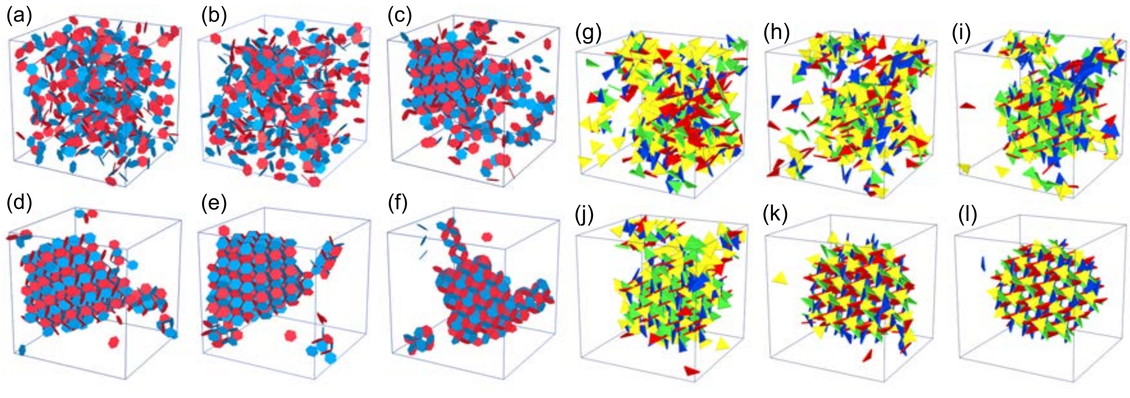

Figure 2 Growth of the truncated octahedral sponge {6,4,|4} and the gyrangle assemblies. For the latter four colors are guides to the eye. Snapshots from simulations showing growth: (a, g) 5×10^6. (b, h) 2.5×10^7. (c, i) 5×10^7. (d, j) 10^8. (e, k) 2×10^8. (f, l) 4×10^8 (MCS).

[1] H. Tanaka, T. Dotera, and S. T. Hyde, *ACS Nano*, **17**, 15371 (2023).