Design economy and assembly of size-programmable triply-periodic polyhedra from addressable nanotriangles

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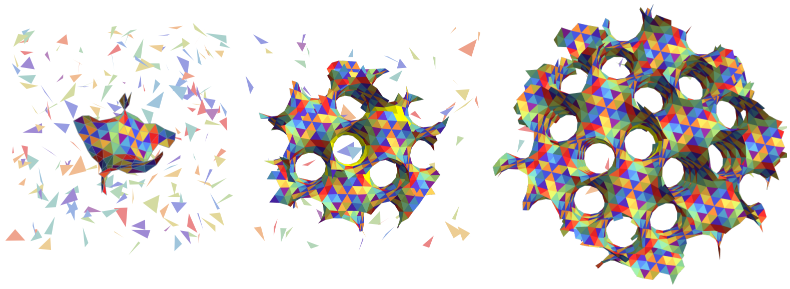

Figure 1 Sequence of snapshots of simulated assemblies of T = 3 Gyroids from programmable triangular subunits, where colors indicate distinct subunit species.

As first suggested by Caspar and Klug [1], many viruses assemble icosahedral shells (capsids) because the high symmetry of the icosahedron enables economical assembly – enclosing a large volume with relatively few distinct protein subunit types. We propose and investigate an extension of the Caspar-Klug symmetry principles for viral capsid assembly to the programmable assembly of size-controlled triply-periodic polyhedral [2], discrete variants of the Primitive, Diamond, and Gyroid cubic minimal surfaces [3]. Inspired by a recent class of programmable DNA origami triangular colloids [4-5], we demonstrate that the economy of design in these crystalline assemblies – in terms of the growth of the number of distinct particle species required with the increased size-scale (e.g. periodicity) – is comparable to viral shells. We further test the role of geometric specificity in these assemblies via dynamical assembly simulations, which show that conditions for simultaneously efficient and high-fidelity assembly require an intermediate degree of flexibility of local angles and lengths in programmed assembly. Off-target misassembly occurs via incorporation of a variant of disclination defects, generalized to the case of hyperbolic crystals. The possibility of these topological defects is a direct consequence of the very same symmetry principles that underlie the economical design, exposing a basic tradeoff between design economy and fidelity of programmable, size controlled assembly. We also present preliminary results of experimental efforts to realize Primitive assemblies from assembly of DNA origami colloids programmable edge binding and geometry.

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