Economical routes to size-specific assembly of self-closing structures

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Triangular monomers with programmable local curvature and specific interactions assemble into self-closing cylindrical tubules. Self-closing assemblies are prone to polymorphism due to the large number of self-closing states with similar energies, such as tubules with different diameter or pitch. Adding complexity, by using multiple unique assembly subunits, can increase the free-energy landscape of off-target structures, improving the yield of a particular assembly outcome (the selectivity). Experimental realizations of tubule assembly show that the selectivity first increases and then plateaus with increasing complexity; the cross-over point denotes the optimal economy for assembly, where one can achieve maximum selectivity using the minimum number of distinct subunit species. A theoretical elastic energy model predicts how this cross-over point depends upon the selfclosing size, the number of unique subunits, and the mechanical properties of the subunit assemblies.

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