Hierarchical assembly is more robust than egalitarian assembly

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Triangular monomers with positive Gaussian curvature and specific interactions assemble into a self-closing icosahedral capsid containing 60 subunits. Brownian Dynamics computer simulations show that the capsid yield is controlled by a balance between the binding strengths of the two specific interactions—one between red and blue edges, and one between white edges. Two specific combinations of the binding energies lead to a dramatic enhancement in the yield, which correspond to two hierarchical pathways: one in which dimers form first and then 30 dimers assemble into the capsid, and one in which pentamers form first and then 12 pentamers assemble into the capsid. These simulations motivate a detailed experimental study of the assembly of synthetic capsids from nanometer-scale subunits made using DNA origami.

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