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A new paradigm for self-assembly: The role of reversibility in viral capsid growth DENNIS RAPAPORT, Bar-Ilan University — The phenomenon of supramolecular self-assembly, despite its importance, remains an enigma. The formation of virus capsids – the exquisitely designed protein shells of spherical viruses – is a well-known example, and there are numerous potential applications for nanotechnology. The capsid assembly process can be modeled using molecular dynamics simulation of simplified particles that are designed to form polyhedral shells. New insights into the mechanism of self-assembly have emerged from simulations carried out using particles immersed in an explicit solvent. Contrary to expectation, self-assembly is found to proceed via a cascade of strongly reversible steps, a feature that helps avoid growth-impeding kinetic traps because partial shells generally tend to lose rather than gain members. This ensures a robust process leading, under suitable conditions, to a high yield of complete shells. Furthermore, despite the large variety of possible intermediate structures, the assembly pathways are found to involve only a small fraction of highly bonded (low energy) forms.

Dennis C. Rapaport
Physics Department, Bar-Ilan University

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