Simulating T=1 and T=3 capsid self-assembly

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Abstract

Viral capsids are known for their high symmetry and exquisite organization, but details of their assembly pathways are not readily accessible, neither theoretically nor experimentally. The nature of such nanoscale construction processes can, however, be explored by molecular dynamics simulations of simple rigid particles designed to form polyhedral shells, in particular the self-assembly of icosahedral shells from triangular particles, and shells corresponding to either T=1 or T=3 capsids from trapezoidal particles. These simulations reveal that under suitable conditions a high yield of complete shells can be obtained, and that successful assembly is attributable to a strongly reversible process which also avoids growth-inhibiting traps. Some aspects of the growth process appear universal, while others depend on particle shape and the size of the product shell. The inclusion of an explicit atomistic solvent proves to be an important element of the simulations. Insight gained from these simplified models has proved helpful in interpreting recent in-vitro experiments.

Keywords: virus, capsid, selfassembly, molecular dynamics

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