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A non-equilibrium model of capsid assembly[1] STEPHEN D. HICKS, C.L. HENLEY, Cornell University — In virus capsids, proteins are assembled into a locally regular triangular lattice (quasiequivalence rule), which permits a variety of possible sizes and shapes (regular or irregular) of the capsid: what selects among these? We present an irreversible growth model in which triangular units are added one at a time. After each addition, we relax the intermediate configurations to minimize a discrete elastic Hamiltonian with in-layer stretching and bending terms. The relaxed angles on the growing edge determine the probability of creating coordination-5 defects, the arrangement of which controls the capsid's global shape; its mean size is controlled by a nonzero preferred inter-unit dihedral angle (spontaneous curvature) included in our Hamiltonian. Using this model, we demonstrate large success rates in forming complete capsids with both deterministic and random growth rules, and measure the degree of icosahedral symmetry of the results. We discuss the assembly of retroviruses, exploring scenarios which give rise to the irregular conical shape of the mature HIV-1 capsid and apply several statistical measures of its deviation from a sphere.

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