Supporting Information

The equilibrium structure of self-assembled protein nano-cages

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NON-EQUILIBRIUM GROWTH MODEL

To simulate the growth of a protein shell under non-equilibrium conditions, we consider equilateral triangles as our building blocks, see Fig. S1. We assume that during the growth process, a shell forms by addition of triangular subunits one at a time, see Ref. [S1] for all the details and justifications of the model. At each step of growth, a new subunit is added to a location on the edge of partially assembled shell, such that it maximizes the number of neighboring triangles. This is achieved by adding the new subunit to the location with the smallest opening angle α, see Fig. S1 (b). As the shell grows, if a vertex already has five neighboring triangles, in the following step either a pentamer forms by joining the two edges or a hexamer assembles by inserting a new subunit, based on which capsomer yields lower energy per subunit in the growing shell, see Fig. S1 (c) and (d). This step is irreversible: a pentamer or hexamer once formed, it cannot dissociate later in the growth process. We let the elastic sheet to relax after each growth step using BFGS method. Figure S2 illustrates intermediate steps of the growth of a $T = 3$ structure. For more details please see Ref. [S1].

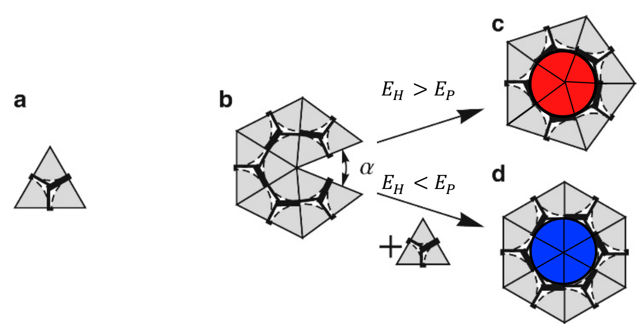

FIG. S1. (a) An equilateral triangular subunit. (b) A new subunit attaches to a location with the smallest opening angle, α. (c) As the shell grows, a pentamer forms by joining the unbound edges if its assembly lowers the energy per subunit in the growing shell, compared to a hexamer. Otherwise, a new subunit will be inserted to construct a hexamer (d) [S1].

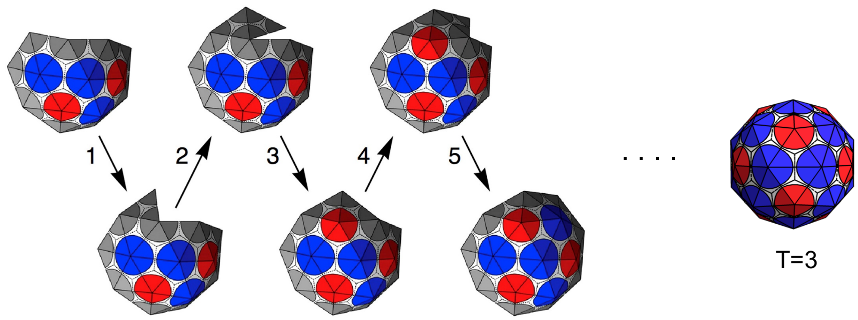

FIG. S2. A series of snapshots of simulations showing the step-by-step growth of a shell: In steps 1 and 2, a new subunit is added at a location with the smallest opening angle. In step 3, two unbound edges are joined, forming a pentamer based on the criteria in Fig. S1 (c). In step 4, one new subunit is added to a location with the smallest opening angle. In step 5, a new subunit is added to construct a hexamer. The growing process leads to the formation of an icosahedral structure $T = 3$. The gray wedges correspond to vertices on the edge, the blue ones to the hexamers and the red ones to the pentamers [S1].

SUPPORTING FIGURES

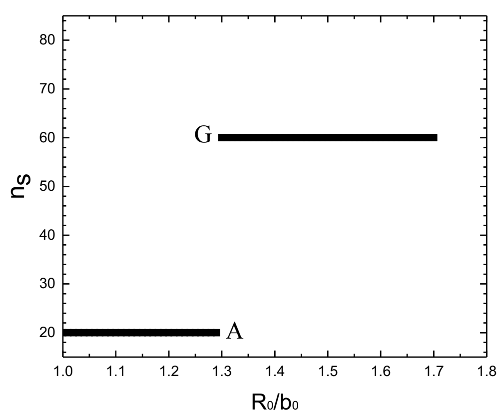

FIG. S3. Plot of number of subunits in the equilibrium structures versus the spontaneous radius of curvature R_0/b_0 at $\gamma = 8$. The two flat lines in the plot correspond to $T = 1$ and $T = 3$ icosahedral structures.

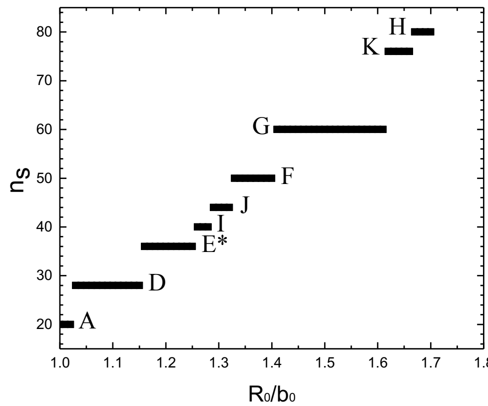

FIG. S4. Number of subunits in the equilibrium structures versus the spontaneous radius of curvature R_0/b at $\gamma = 0.2$. The label next to each line shows the associated structure, illustrated in Fig. 5 in the paper.

[S1] J. Wagner and R. Zandi, Biophysical journal **109**, 956 (2015).