Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information for
Effect of coat-protein concentration on the self-assembly of bacteriophage MS2 capsids around RNA†

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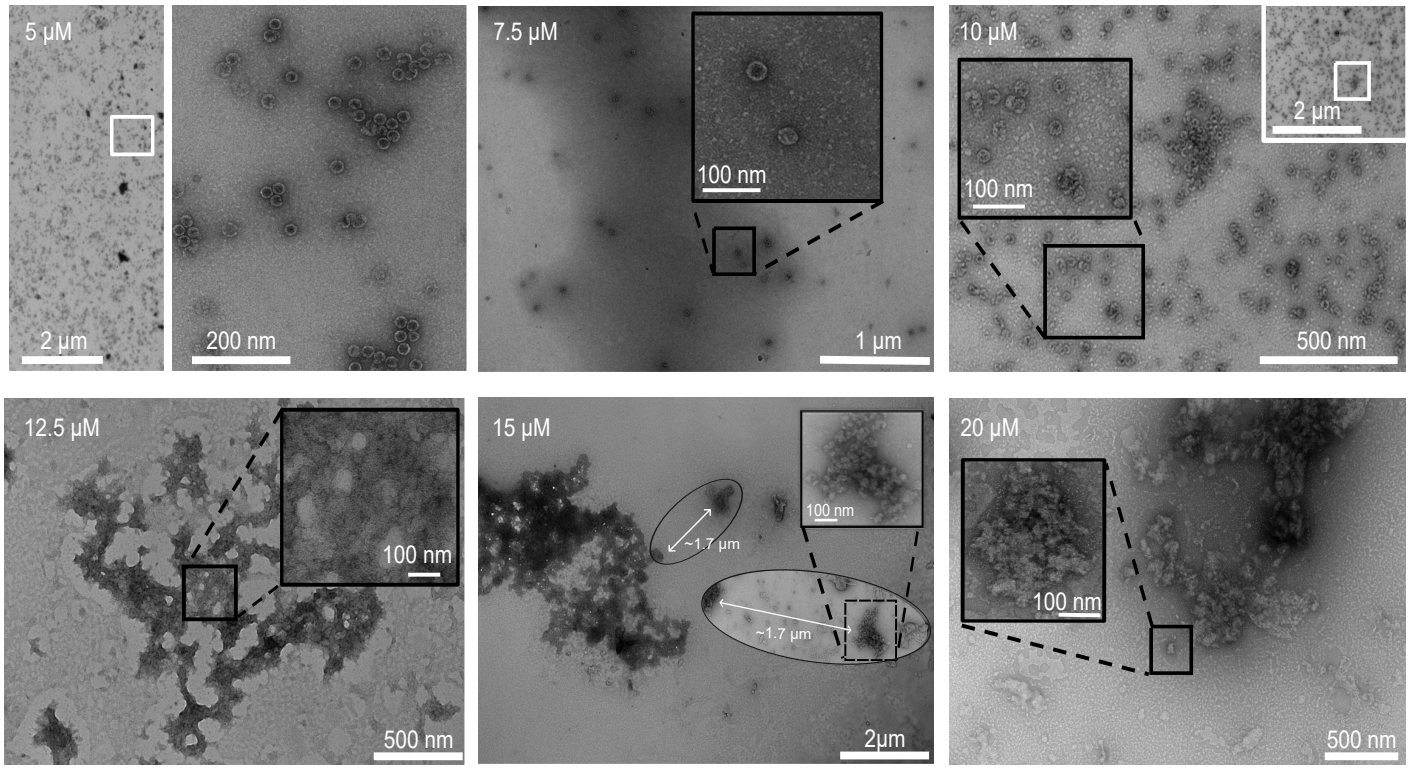

Fig. S1 TEM images of the same samples as shown in Fig. 4, but at different magnifications for each sample (some rotation and translation may be present between the low-magnification images and the insets due to drift in the microscope). The low magnification images of the samples at 12.5 μM coat-protein dimer concentration and higher show micrometer-sized structures.

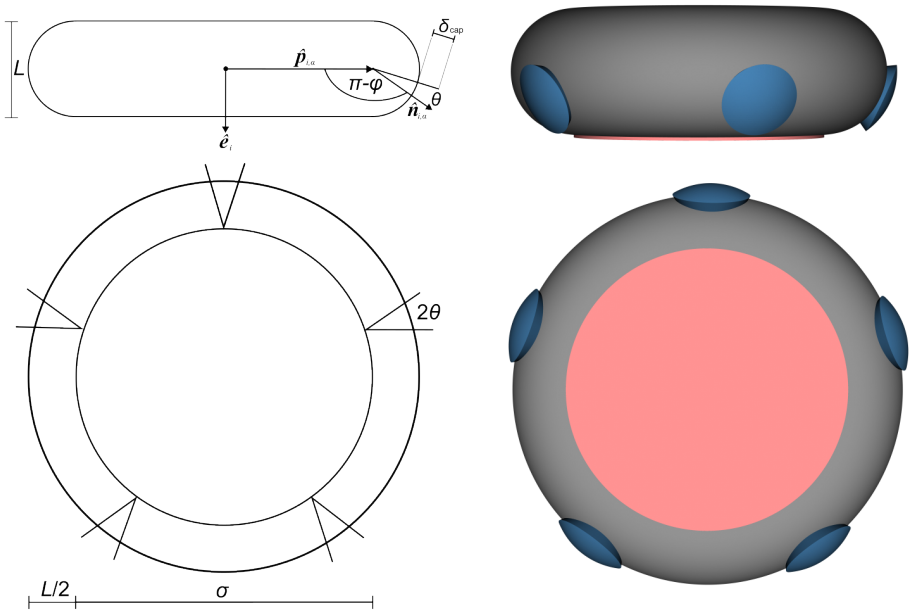

Fig. S2 Schematic (left) and three-dimensional (right) representation of the patchy particle model for capsomers. The schematic view of the model shows key model parameters that define the geometry of the hard core of each capsomer particles, namely the diameter σ and thickness L. Additionally, parameters that define the geometry of the attractive patches are shown for one of the five patchy sites, where $\hat{\mathbf{p}}_{i,\alpha}$ defines the position of the patch in the local coordinate frame of the capsomer, $\hat{\mathbf{n}}_{i,\alpha}$ is the vector defining the orientation of the patch, θ is the half-angle of the patch, φ is the angle between $\hat{\mathbf{n}}_{i,\alpha}$ and the plane containing the circular core of the capsomer and δ_{cap} is the range of the attractive patch-patch interactions. We show a three-dimensional representation of the particles used in this work on the right.

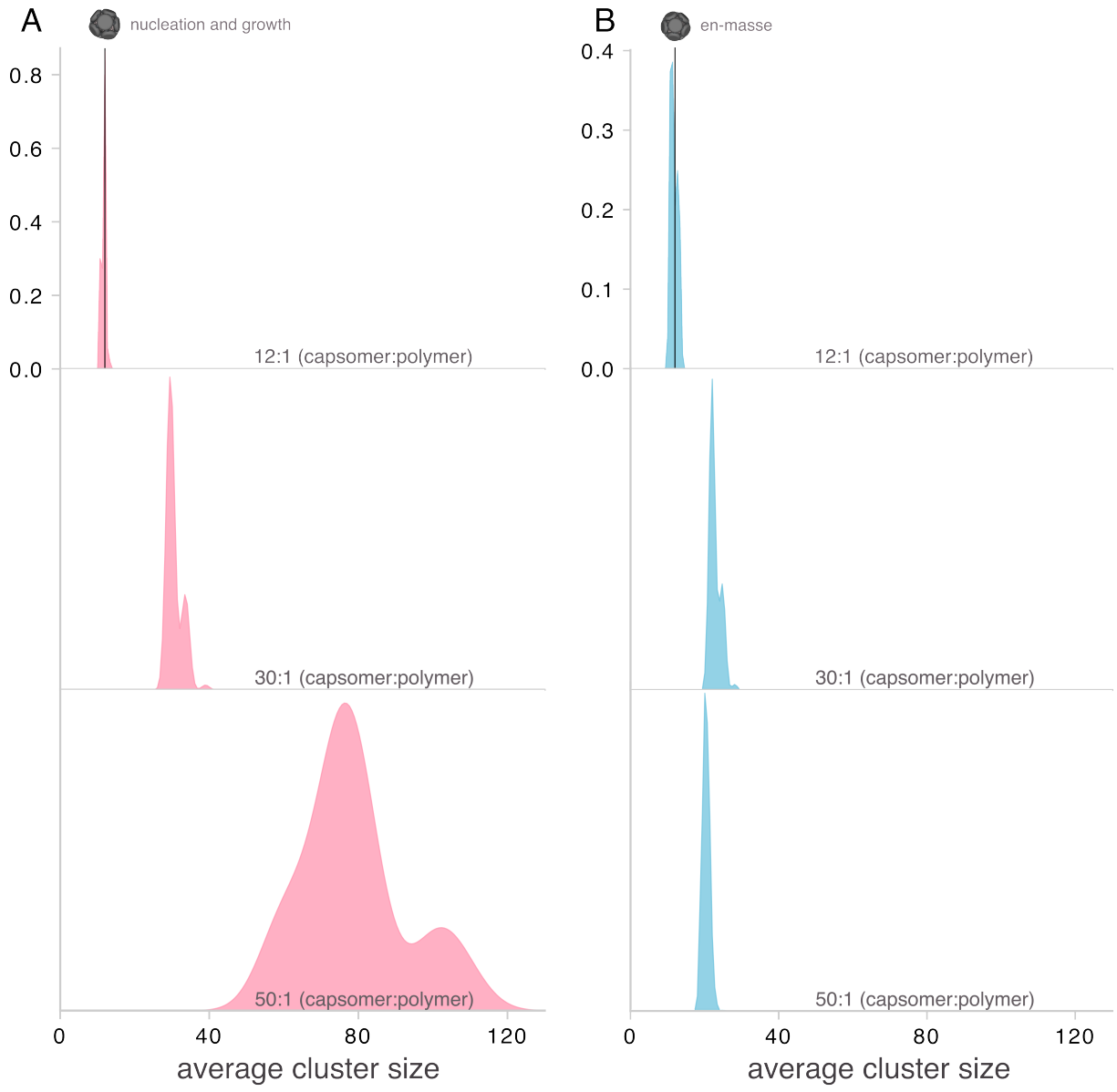

Fig. S3 Average cluster size distributions observed in Monte Carlo simulations of capsomer-and-polymer systems where the relative energies of capsomer-capsomer and capsomer-polymer interactions are chosen such that capsid formation in the low capsomer:polymer ratio systems proceeds either by (A) a nucleation and growth pathway or (B) an en-masse pathway. For both sets of simulations, the average cluster sizes are computed for systems containing 12:1, 30:1 and 50:1 ratio of capsomer to polymer.

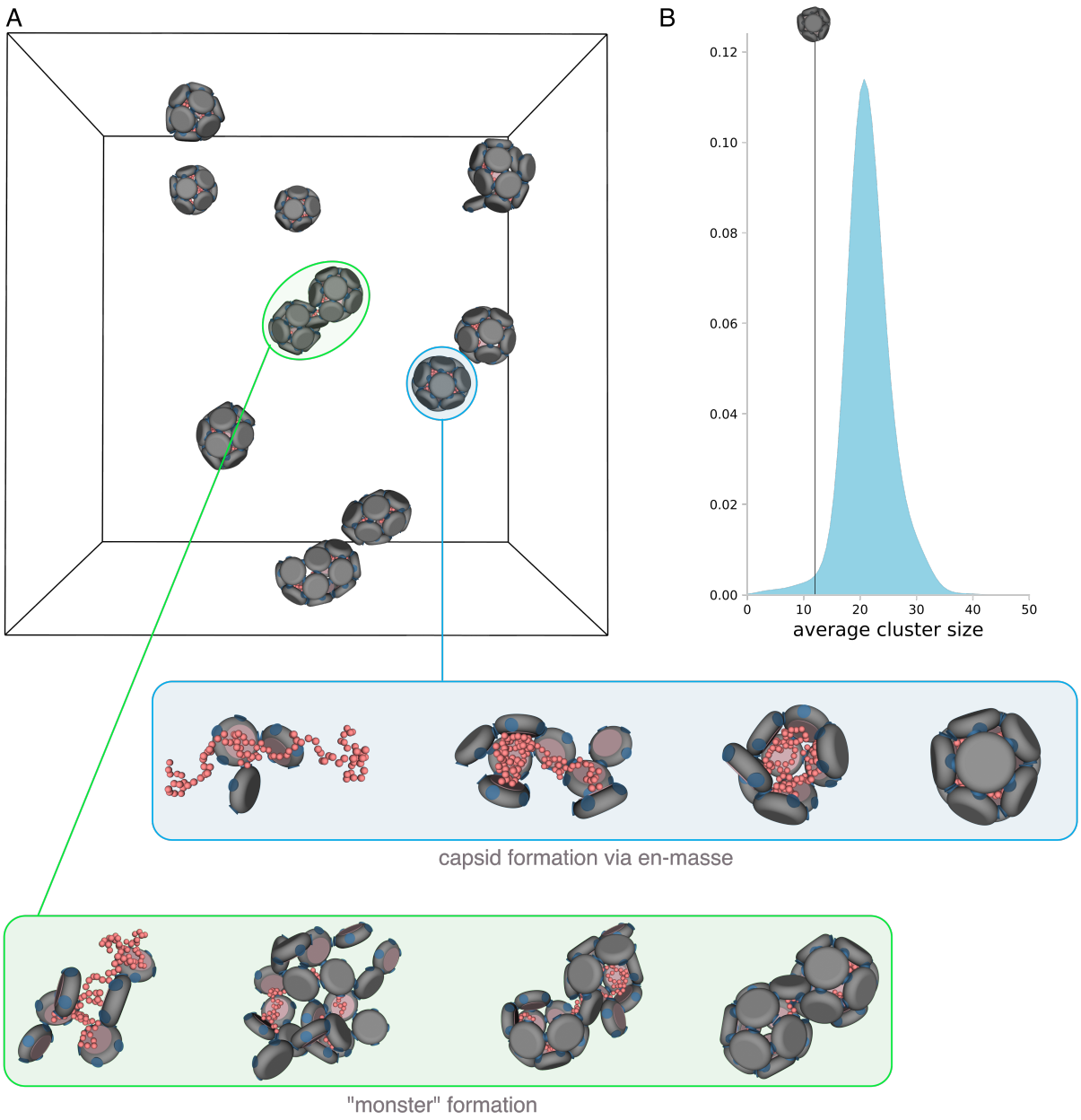

Fig. S4 Results of Monte Carlo simulations at a high capsomer:polymer ratio (50:1) with short polymer chains and capsomer-capsomer and capsomer-polymer interactions chosen such that capsids nucleate and grow in the low capsomer:polymer ratio systems. (A) Representative snapshot of clusters that contain polymer chains. Two clusters have been highlighted. One is a monster particle that forms when two capsid shells assemble around a single polymer chain, and the other is a capsid that assembles *via* an en-masse pathway, as shown in the shaded boxes. (B) Average cluster size distribution for the system, showing that when the polymer chains are short, the system contains no condensates, and only capsids and monsters form.