Supplemental Material: Spontaneous crumpling of active spherical shells

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I. CROSS-SECTIONS OF ACTIVE ELASTIC SHELLS

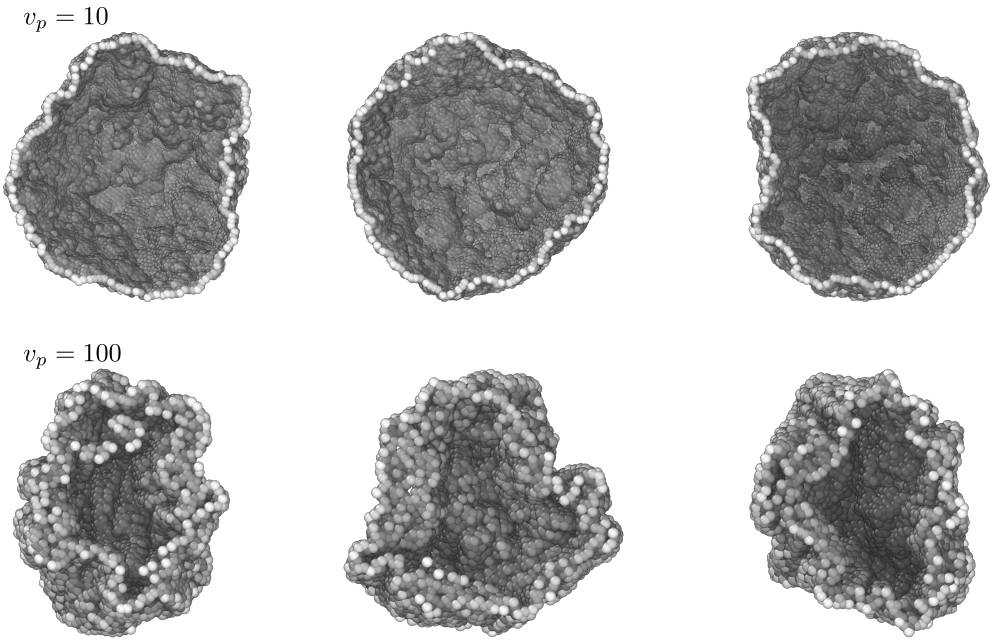

FIG. SI.1. Cross-sections of active elastic shells at $v_p = 10$ (top row) and $v_p = 100$ (bottom row). The perspectives are along three orthogonal axis. The elastic constants are $K = 160\,k_{\rm B}T_0/\sigma^2$ and $\kappa = 10\,k_{\rm B}T_0$ and the size of the amorphous shell is $N = 12002$.

II. DISCRETIZING THE LAPLACIAN OPERATOR TO IMPLEMENT BENDING ENERGY

When the shell is discretized using flat triangles, bending forces can be calculated using two methods - referred to as Method A and B [1, 2]. For all numerical calculations, we implemented Method A where we calculate the angle between normals of neighboring triangles (see Eq. 1 of the main text). To ensure that the collapse of normalized volumes of the shells as a function of $v_p/(K^{0.125}\kappa^{0.5})$ is not a numerical artefact of our choice of using Method A, in this section, we present some results where we calculate bending forces using Model B [2, 3]. For a membrane whose local mean curvature at $\boldsymbol{r}$ is $H(\boldsymbol{r})$, the height field is $h(\boldsymbol{r})$ and the bending constant is $\tilde{\kappa}$, the Helfrich bending energy is,

$$E_{\rm bend} = \frac{\tilde{\kappa}}{2}\int dA\, H(\boldsymbol{r})^2 \approx \frac{\tilde{\kappa}}{2}\int dA\, [\nabla^2 h(\boldsymbol{r})]^2. \tag{SI.1}$$

For a triangulated surface, whose node positions are denoted by $\boldsymbol{r}_i$, the discretized form of the Laplacian allows the mean curvature at the $i^{\rm th}$ vertex to be calculated as,

$$H_i = \frac{1}{\sigma_i}\boldsymbol{n}_i \cdot \sum_j \sigma_{ij}\frac{\boldsymbol{r}_{ij}}{r_{ij}}, \tag{SI.2}$$

where index j denotes the neighboring vertices of i, $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $r_{ij} = |\boldsymbol{r}_{ij}|$, $\boldsymbol{n}_i$ is the surface normal and σ_i is the area of the virtual dual cell of vertex i,

$$\sigma_i = \frac{1}{4}\sum_j \sigma_{ij} r_{ij}. \tag{SI.3}$$

The length σ_{ij} is,

$$\sigma_{ij} = \frac{r_{ij}}{2}[\cot(\theta_1) + \cot(\theta_2)], \tag{SI.4}$$

where θ_1 and θ_2 are opposing angles of the two triangles sharing the bond ij. See Fig. SI.2(a). The discretized bending energy we use in our simulations is,

$$E_{\text{bend}} = \frac{\tilde{\kappa}}{2}\sum_i \frac{1}{\sigma_i}\left[\boldsymbol{n}_i \cdot \sum_j \sigma_{ij}\frac{\boldsymbol{r}_{ij}}{r_{ij}}\right]^2. \tag{SI.5}$$

In Fig. SI.2(b), we see that the collapse of the normalized volumes as a function of $v_p/(K^{0.125}\tilde{\kappa}^{0.5})$ is retained despite the use of an alternate implementation of bending energy.

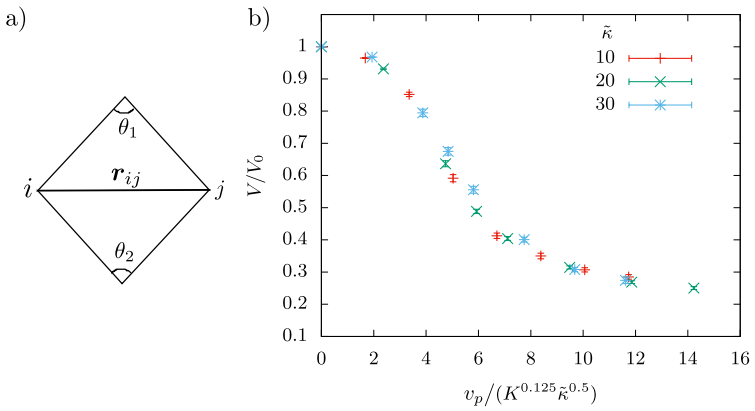

FIG. SI.2. a) Sketch of two flat triangles sharing a bond. b) The elastic stretching constant $K = 160$ and the size of the crystalline shell is $N = 1922$.

III. CRUMPLED ACTIVE SHELLS RESWELL ON REMOVAL OF ACTIVITY

Elastic shells buckle at high temperatures of $T = 100\,T_0$, yet do not display a crumpled phase as we verified. To check the stability of the crumpled phase at high temperatures, we use a crumpled configuration as the initial configuration for a shell in a thermal bath of high temperature. Specifically, the initial configuration was generated by subjecting the shell to active fluctuations of strength $v_p = 100$ at $T = T_0$ after which the activity was removed and the temperature is increased to $T = 100\,T_0$. The shell immediately reswells to a volume of $V \approx 0.6\,V_0$. See Fig. SI.3. This suggests that a crumpled phase of the elastic shell is not stable even under these high temperatures.

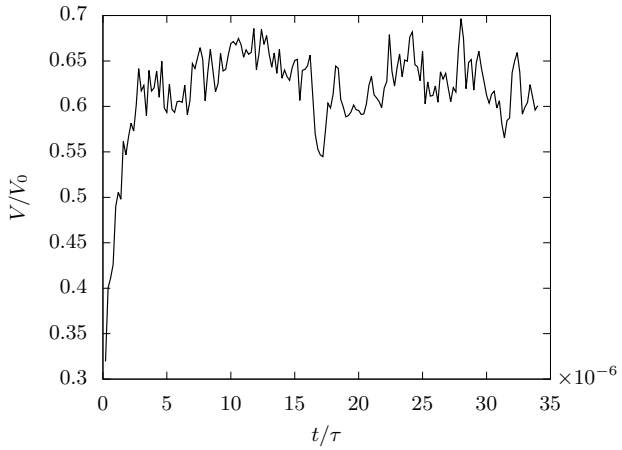

FIG. SI.3. Normalized volume V/V_0 as a function of time depicting the reswelling of a crumpled configuration. The elastic constants are $K = 160\, k_B T_0/\sigma^2$ and $\kappa = 10\, k_B T_0$ and the size of the amorphous shell is $N = 1922$.

IV. FINITE SIZE DEPENDENCE

A. Radius of gyration

At every self-propulsion speed v_p, the radius of gyration R_g must scale with radius of spherical shell R as $R_g(v_p) \sim R^{\nu(v_p)}$ where the size exponent $\nu(v_p)$ is numerically calculated in Fig. 4 of the main text. For $v_p = 100$, the size dependence of the radius of gyration is shown in Fig. SI.4 where the best fit for data is at $\nu(100) = 0.83 \pm 0.03$. The error bar is the fitting error.

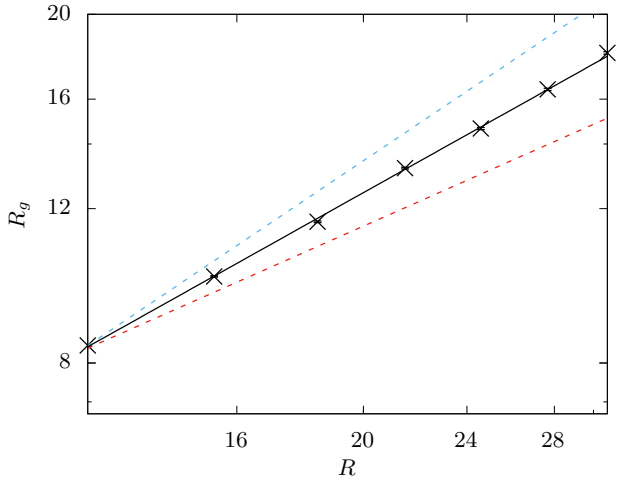

FIG. SI.4. At a self-propulsion speed of $v_p = 100$, the radius of gyration of active crystalline shells scales with shell radii as $R_g \sim R^\nu$ with $\nu = 0.83 \pm 0.03$. In this log-log plot, the dashed blue and red lines are for reference and show the size scaling of the flat phase and compact phase respectively. The small error bars on the data are standard errors.

B. Normalized volumes

If the volume $V(v_p)$ of the shell is approximated as $V(v_p) \sim R_g^3(v_p)$, then

$$\frac{V(v_p)}{V_0} \approx \frac{R_g^3(v_p)}{R^3} = R^{3[\nu(v_p)-1]}. \tag{SI.6}$$

For small self propulsion speeds, $\nu(v_p) - 1 \approx 0$ and following Eq. SI.6, the normalized volume curves should exactly overlap irrespective of size of the shell. See Fig. 1 of main text. With increasing v_p, $\nu(v_p) - 1$ monotonically decreases as seen in Fig. 4 of main text. Thus, following Eq. SI.6, the normalized volumes $V(v_p)/V_0$ become more size dependent with increasing v_p. Correspondingly, the spread of the normalized volume curves of different sizes is seen to increase with increasing v_p as can be seen in Fig. 1 of the main text.

V. PRESSURE INDUCED COLLAPSE OF SHELLS

Passive shells can be collapsed with sufficient negative i.e. inward pressures. To find qualitative differences between activity-induced collapse and pressure-induced collapse, we calculate the size exponent of shells that are collapsed using negative pressures. For this elastic shell under the influence of pressure p, we perform Monte Carlo simulations using the interaction potential,

$$U_p = K_s \sum_{<ij>} \Theta(r_{ij} - l_0) + \kappa \sum_{<lm>} (1 - \boldsymbol{\eta}_l \cdot \boldsymbol{\eta}_m) - pV + 4\,\varepsilon \sum_{ij} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} + \frac{1}{4} \right]. \tag{SI.7}$$

All variable definitions are as defined under Eq. 1 of the main text. The Heaviside step function $\Theta(x) = 1$ for $x \geq 0$ and zero otherwise while the constant $K_s \to \infty$.

To collapse the shell, we use a large pressure $p/p_c = 200$ for all sizes, where the critical pressure for buckling scales with shell radius as $p_c \sim 1/R^2$ [4]. With the shell in a thermal bath of temperature $T = T_0$, we relax the shell until the radius of gyration saturates to a constant value after which we calculate the average radius of gyration R_g. See Fig. SI.5(a) shows the typical shape of highly compressed elastic shells. The scaling of the radius of gyration with shell radii is $R_g \sim R^\nu$ with $\nu = 1.00 \pm 0.03$. The error bar is the fitting error. See Fig. SI.5(b) where we show the averaged data for twenty independent runs. The shell despite its complete collapse scales linearly with shell radii in contrast to active shells that remain in the crumpled phase at high self-propulsion speeds.

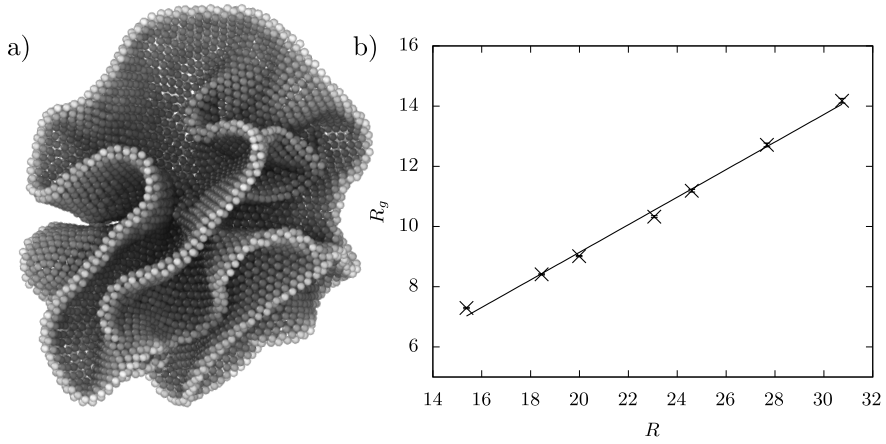

FIG. SI.5. a) Snapshot of a pressure collapsed crystalline shell of size $N = 12002$. b) At a large inward pressure of $p/p_c = 200$, the radius of gyration scales with the shell radii as $R_g \sim R^\nu$ with $\nu = 1.00 \pm 0.03$. The small error bars on the data are standard errors. Note that both axes in the plot are linear.

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