Supplementary Information for Chemically Controlled Shape-morphing of Elastic Sheets

Raj Kumar Manna[1], Oleg E. Shklyaev[1], Howard A. Stone[2], Anna C. Balazs[1]*
[1]Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA 15260, USA
[2]Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA

Elastic energy of the sheet

The elastic sheet is modeled as a two dimensional network of active nodes that are connected by elastic bonds (white lines in Fig. 1a of main text). The elastic energy of the connected bonds are modeled as Kirchhoff's rod[1]

$$E = \frac{1}{2}\kappa_s \int \left[\left(\mathbf{D}_1 \cdot \frac{d\mathbf{r}}{ds} - 1 \right)^2 + \left(\mathbf{D}_2 \cdot \frac{d\mathbf{r}}{ds} - 1 \right)^2 + \left(\mathbf{D}_3 \cdot \frac{d\mathbf{r}}{ds} - 1 \right)^2 \right] ds + \frac{1}{2}\kappa_b \int \left[\left(\frac{d\mathbf{D}_2}{ds} \cdot \mathbf{D}_3 \right)^2 + \left(\frac{d\mathbf{D}_3}{ds} \cdot \mathbf{D}_1 \right)^2 + \left(\frac{d\mathbf{D}_1}{ds} \cdot \mathbf{D}_2 \right)^2 \right] ds \quad \text{(S1)}$$

where κ_s and κ_b are respectively stretching and bending modulus of the rod. $\mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3$ are the unit orthonormal directors at each node of the sheet and *s* is the contour length along the sheet.

Transition from the self-folded state to a dome-like state

The different shape-morphing structures are characterized by the Gaussian and mean curvatures. With two principle curvatures of κ_1 and κ_2 of a surface patch, the Gaussian curvature (K) and mean curvature (H_C) are defined as $K = \kappa_1 \kappa_2$ and $H_C = (\kappa_1 + \kappa_2)/2$, respectively. The mean and Gaussian curvatures at each node of the elastic sheet are computed using a model of discretized surfaces[2]. The average mean curvature ($\langle H_C \rangle$) of any shape is computed by taking average over all the node of the sheet. The transition from the self-folded state to a dome-like state with increasing elasticity (i.e., increasing bending modulus κ_b while keeping stretching modulus, κ_s fixed) is evident from the average mean curvature (Fig. S1). The bending modulus at which this transition occurs decrease with an increase in the stretching modulus, κ_s, of the elastic sheet (Fig. S1). Notably, these different states are obtained for a constant maximal reaction rate, $r_{m,\text{sheet}}^{\text{enzyme}}$. Alternatively, different 3D structures and transitions from the self-folded to dome-like states can also be obtained by fixing the bending modulus and varying the maximal reaction rate of enzyme (Fig. S2).

Supplementary figures

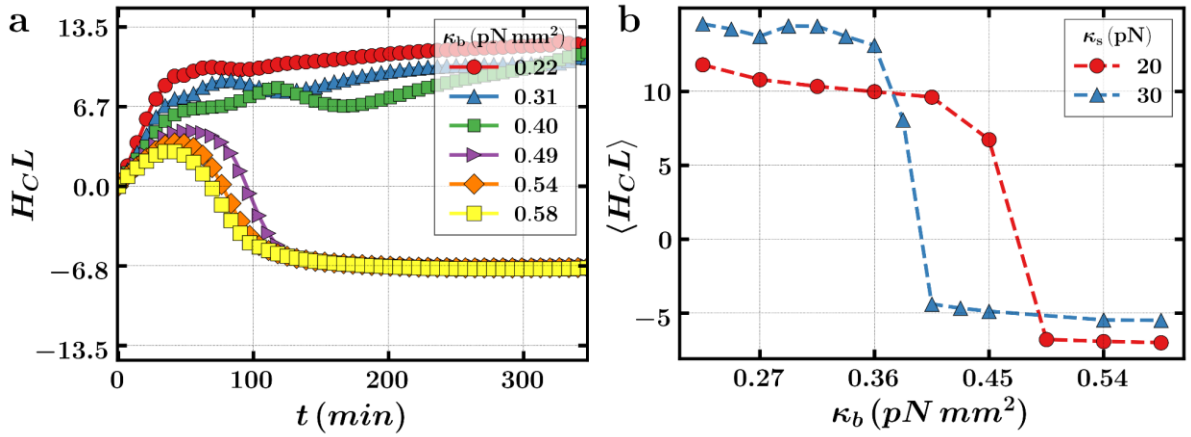

Figure S1. Mean curvature of the catalase-coated elastic sheet. (a) Evolution of scaled mean curvature ($H_C L$) of the catalase-coated elastic sheet (Fig. 1a) with time for different values of elastic parameter (bending modulus, κ_b). The time variation of mean curvatures indicates transition from positive mean curvature (corresponds to self-folding state) to negative mean curvature (corresponds to dome-like state) as bending modulus is increased. This transition from self-folded state to dome-like sate is also evident from the variation of average mean curvature with bending modulus, κ_b (b). The bending modulus at which this transition occur decreases with the increase of stretching modulus κ_s.

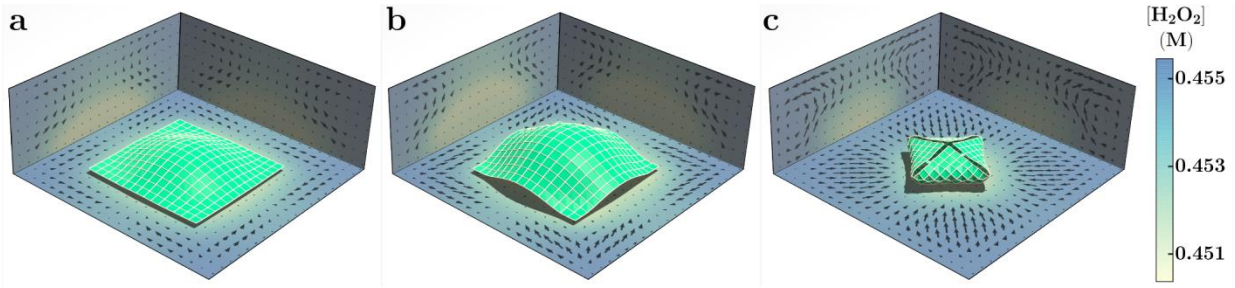

Figure S2. Transition of the sheet's shape $h(x,y,t)$ from dome-like state to self-folded state by fixing the bending modulus, κ_b, and varying the maximal reaction rate of rate of catalase-catalyzed reaction. The maximal reaction rates corresponding to the configuration (a-c) are $r_{m,\mathrm{sheet}}^{\mathrm{CAT}} = 2.6\times10^{-6}\,\mathrm{mol\,m^{-2}\,s^{-1}}$, $r_{m,\mathrm{sheet}}^{\mathrm{CAT}} = 4.7\times10^{-6}\,\mathrm{mol\,m^{-2}\,s^{-1}}$ and $r_{m,\mathrm{sheet}}^{\mathrm{CAT}} = 5.2\times10^{-6}\,\mathrm{mol\,m^{-2}\,s^{-1}}$ respectively (c). The bending and stretching moduli of the sheet are $\kappa_b = 0.22\,\mathrm{pN\,mm^2}$ and $\kappa_s = 20\,\mathrm{pN}$ respectively. The configurations of the elastic sheet are at 375 minutes after the start of the catalytic reaction.

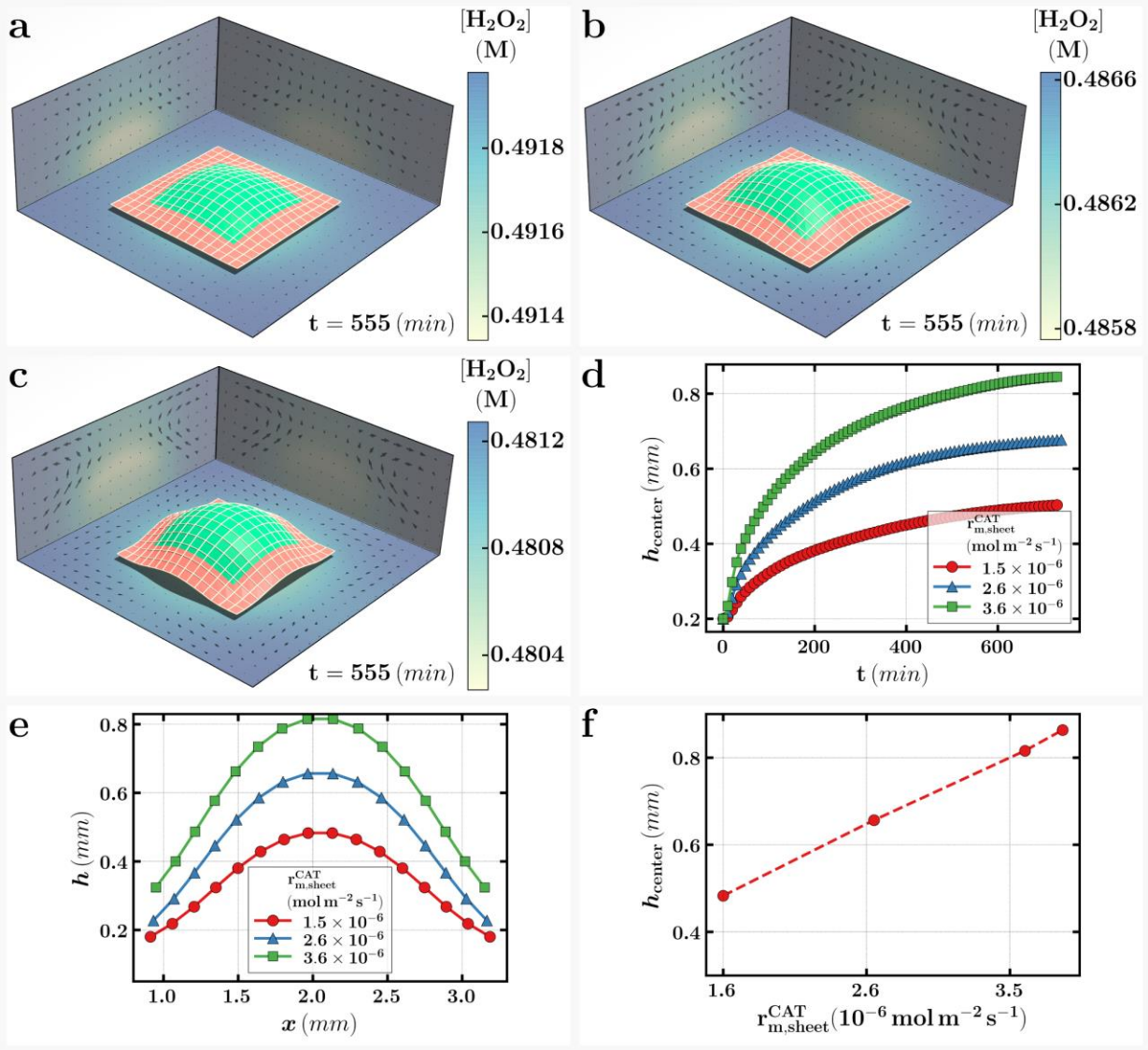

Figure S3. Controlling the height $h(x, y, t)$ of the dome-like state by varying maximal reaction rate of catalase-catalyzed reaction. The configurations of the dome-like shape for maximal reaction rates $r^{\mathrm{CAT}}_{m,\mathrm{sheet}} = 1.5\times10^{-6}\ \mathrm{mol\ m^{-2}\ s^{-1}}$ (a), $r^{\mathrm{CAT}}_{m,\mathrm{sheet}} = 2.6\times10^{-6}\ \mathrm{mol\ m^{-2}\ s^{-1}}$ and $r^{\mathrm{CAT}}_{m,\mathrm{sheet}} = 3.6\times10^{-6}\ \mathrm{mol\ m^{-2}\ s^{-1}}$ (c). The configurations of the elastic sheet in (a-c) are at 555 minutes after the start of the catalytic reaction. (d) Time evolution of the height of the center of the sheet shows the system reaches in a quasi-static state. (e-f) The height of center $h(L/2, L/2, t)$ of the dome-like state is increased with the increase of maximal reaction rate for catalase-catalyzed reaction. This is quantified by computing the height profile $h(x, L/2, t)$ of the middle of the sheet (e) for different maximal reaction rates and the variation of height of the center of the sheet with $r^{\mathrm{CAT}}_{m,\mathrm{sheet}}$ (f). The instantaneous height in (e-f) are at 555 minutes after the start of the catalytic

reaction. The bending and stretching moduli of the sheet are $\kappa_b = 0.22\,\mathrm{pN\,mm^2}$ and $\kappa_s = 20\,\mathrm{pN}$ respectively.

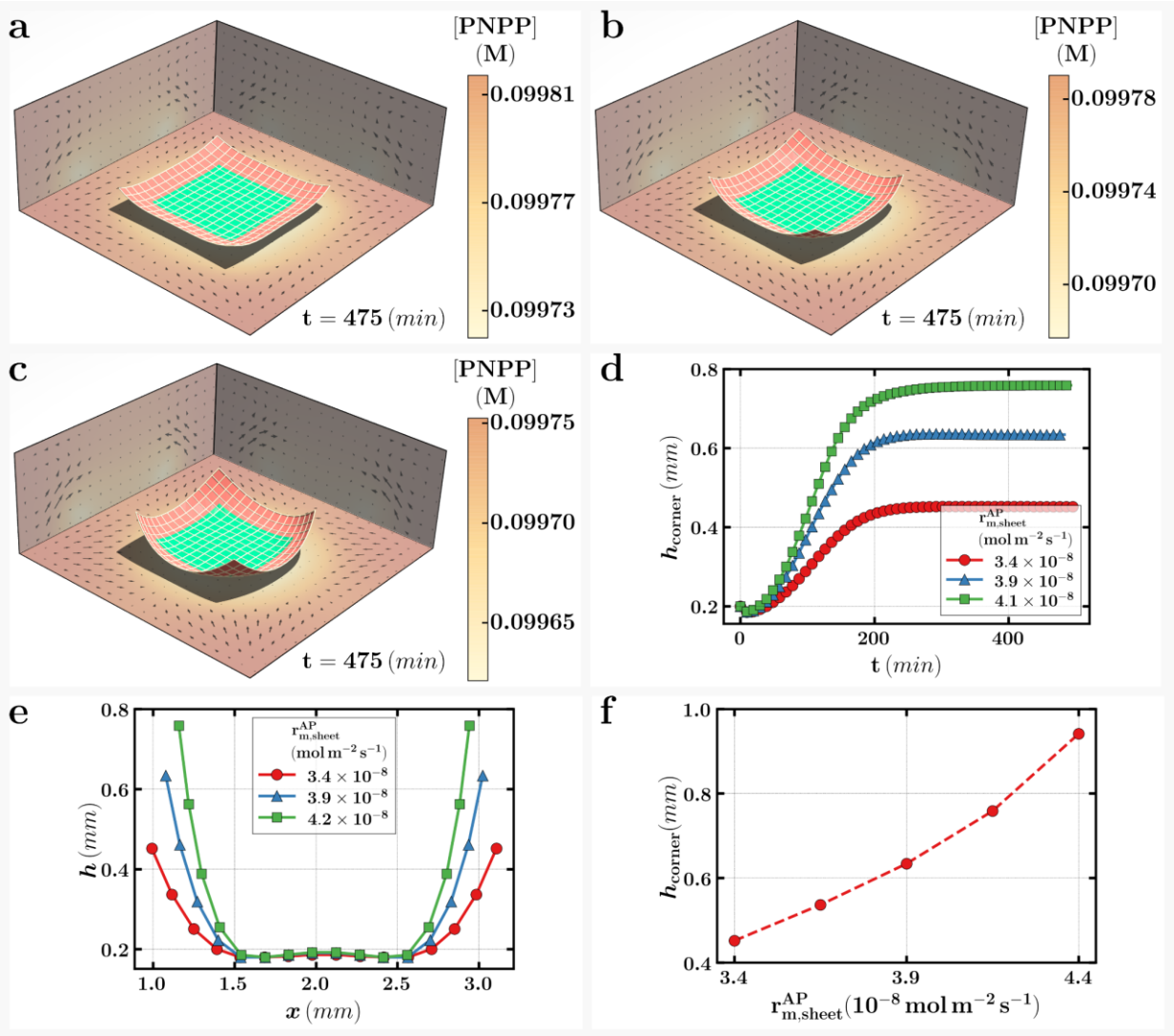

Figure S4. Controlling the curvature of bowl-like state by varying maximal reaction rate of AP-catalyzed reaction. The configurations of the bowl-like shape for maximal reaction rates $r^{\mathrm{AP}}_{m,\mathrm{sheet}} = 3.4\times10^{-8}\,\mathrm{mol\,m^{-2}\,s^{-1}}$ (a), $r^{\mathrm{AP}}_{m,\mathrm{sheet}} = 3.9\times10^{-8}\,\mathrm{mol\,m^{-2}\,s^{-1}}$ and $r^{\mathrm{AP}}_{m,\mathrm{sheet}} = 4.2\times10^{-8}\,\mathrm{mol\,m^{-2}\,s^{-1}}$ (c). The configurations $h(x,y,t)$ of the elastic sheet in (a to c) are at 475 minutes after the start of the catalytic reaction. (d) Time evolution of the height of a corner of the sheet shows the system reaches in a quasi-static state. The curvature of the bowl-like state is increased with the increase of maximal reaction rate for AP-catalyzed reaction. This is quantified by computing height profile of a diagonal of the sheet (e) for different maximal reaction rates and the variation of height of a corner with $r^{\mathrm{AP}}_{m,\mathrm{sheet}}$ (f). The instantaneous height in (e-f) are at 475

minutes after the start of the catalytic reaction. The bending and stretching moduli of the sheet are $\kappa_b = 0.22\,\mathrm{pN\,mm^2}$ and $\kappa_s = 20\,\mathrm{pN}$ respectively.

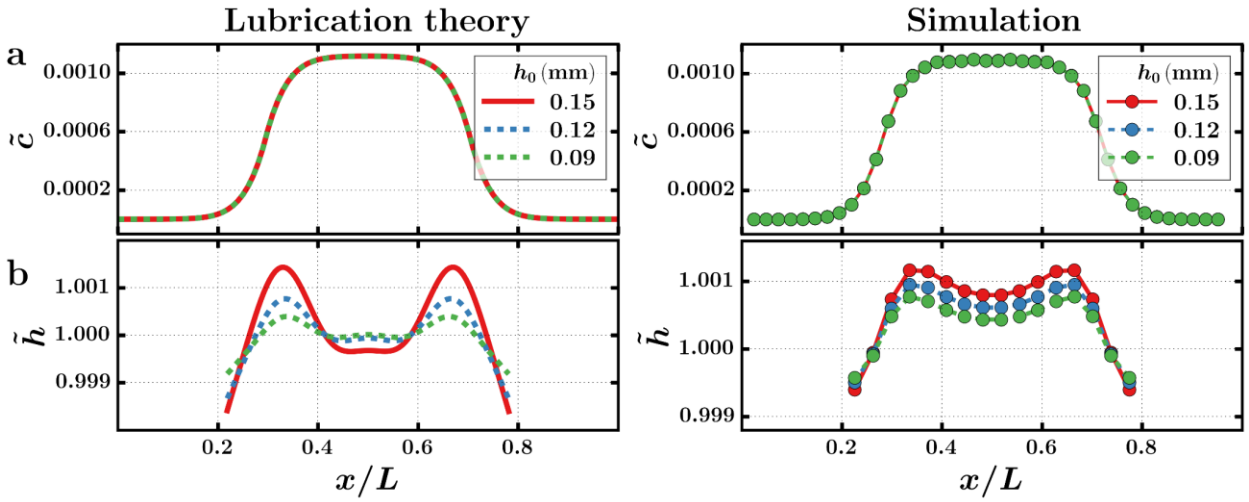

Figure S5. Comparison of initial dynamics of the elastic sheet obtained with the lubrication approximation (left panels) and simulations (right panels) for three initial sheet locations h_0 =0.15 mm, 0.12 mm and 0.09 mm. (a) The top panels show the variation of concentration along the chamber at the physical time t=25s. (b) The profiles of the elastic sheet obtained with the lubrication model (left panels) and simulations (right panels). The closer the sheet is initially located to the bottom wall, the slower is the rate of sheet's deformations and departure from the bottom wall.

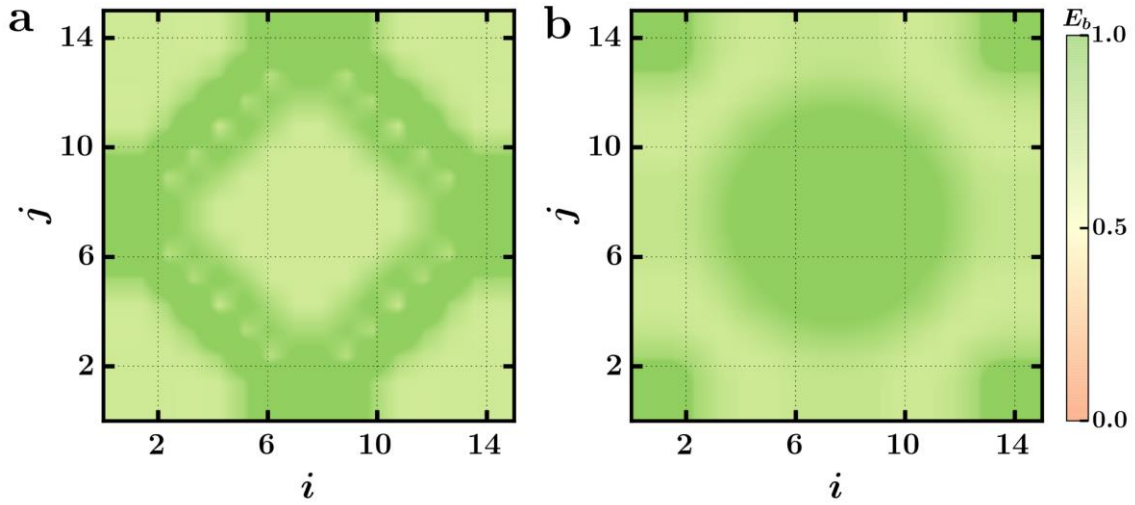

Figure S6. The distribution of bending energy corresponding to the envelope-like structure of Fig. 1(c) and dome-like structure of Fig. 1(d) are plotted in (a) and (b), respectively. The color bar indicates the bending energy normalized by its maximum magnitude. The bending energy is computed from the mean curvature (H_C) as $E_b = \frac{1}{2}\kappa_b \int H_C^2\, ds$.

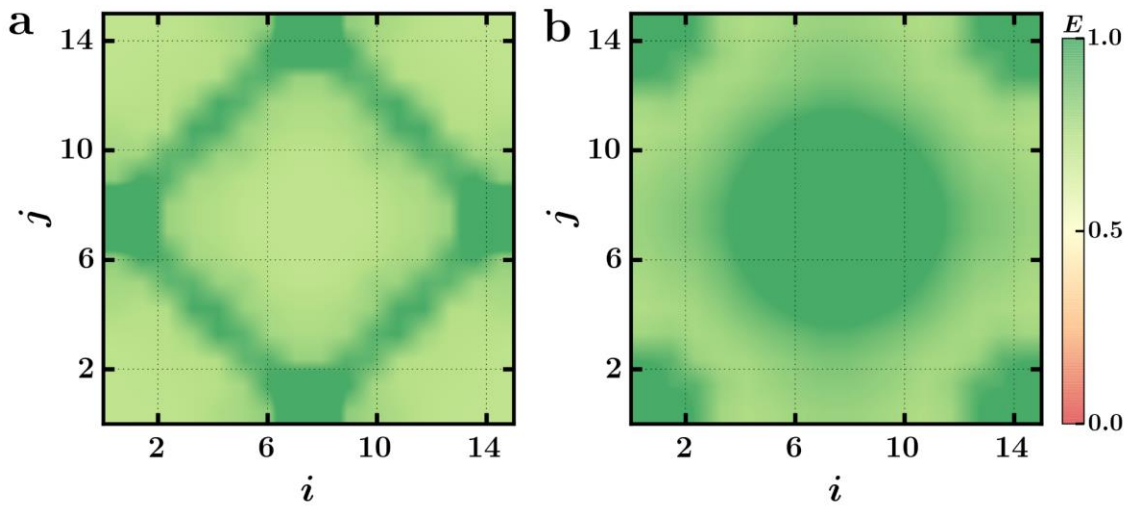

Figure S7. The distribution of elastic energy corresponding to the envelope-like structure of Fig. 1(c) and dome-like structure of Fig. 1(d) are plotted in (a) and (b), respectively. The color bar indicates the elastic energy normalized by its maximum magnitude. The elastic energy is the sum of the bending and stretching energies and is computed according to Eq. (S1).

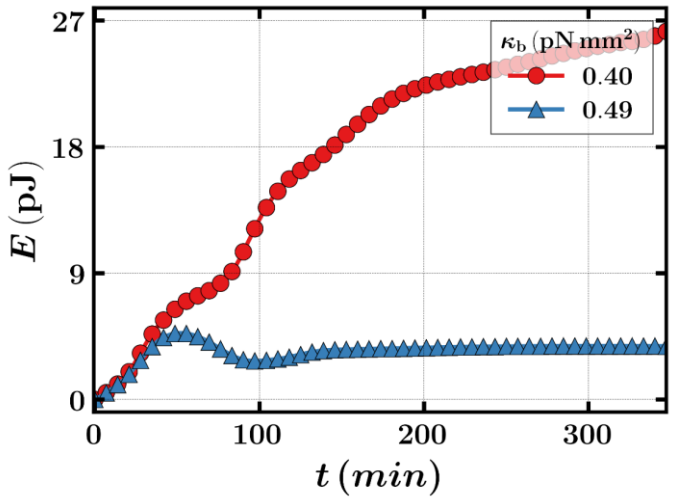

Figure S8. The time evolution of the elastic energy of the sheet corresponding to the parameters of the envelope-like structure of Fig. 1(c) and dome-like structure of Fig. 1(d) are plotted with red and blue symbols, respectively. The elastic energy of the envelope-like state is higher than that of the dome-like state.

References

(1) Lim, S.; Ferent, A.; Wang, X. S.; Peskin, C. S. Dynamics of a Closed Rod with Twist and Bend in Fluid. *SIAM J. Sci. Comput.* **2008**, *31* (1), 273–302.

(2) Nelson, David R and Piran, Tsvi and Weinberg, S. *Statistical Mechanics of Membranes and Surfaces*; 2004.