Supplementary Material for:

Geometric coupling of helicoidal ramps and curvature-inducing proteins in organelle membranes

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S1 Local force balance of elastic surfaces at mechanical equilibrium

The equation of mechanical equilibrium of an elastic surface ω subject to a lateral pressure p can be written in the compact form

$$\mathbf{\Sigma}^{\alpha}_{;\alpha} + p\mathbf{n} = \mathbf{0} \ , \tag{S1}$$

where $\mathbf{\Sigma}^{\alpha}$ are the stress vectors and $\mathbf{n}$ is the unit normal to the local surface. Greek indices range over $1, 2$, and if repeated, are summed over this range. Semicolon identifies covariant differentiation with respect to the surface metric $a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta$ where $\mathbf{a}_\alpha = \mathbf{r}_{,\alpha}$ are the tangent vectors and $\mathbf{r}(\theta^\alpha)$ is the parametrization of the position field. The commas refer to partial derivatives with respect to the surface coordinates θ^α. With these definitions, the normal vector is given by $\mathbf{n} = (\mathbf{a}_1 \times \mathbf{a}_2)/ \mid \mathbf{a}_1 \times \mathbf{a}_2 \mid$. In Eq. S1, the differential operation represents the surface divergence defined as $\mathbf{\Sigma}^{\alpha}_{;\alpha} = (\sqrt{a})^{-1}(\sqrt{a}\mathbf{\Sigma}^\alpha)_{,\alpha}$ where $a = \det(a_{\alpha\beta})$. In surface theory, a manifold is described by the metric $a_{\alpha\beta}$ defined above, and the curvature tensor given by $b_{\alpha\beta} = \mathbf{n} \cdot \mathbf{r}_{,\alpha\beta}$.

For an elastic membrane whose energy surface density per unit mass depends on the metric and curvature only $F(a_{\alpha\beta}, b_{\alpha\beta}; \theta^\alpha)$, the stress vectors involved in the local force balance (Eq. S1) can be written as [1]

$$\mathbf{\Sigma}^\alpha = \mathbf{T}^\alpha + S^\alpha \mathbf{n} \ . \tag{S2}$$

Here the tangential stress vectors are

$$\mathbf{T}^\alpha = T^{\beta\alpha}\mathbf{a}_\beta \quad \text{with} \quad T^{\beta\alpha} = \Sigma^{\beta\alpha} + b^\beta_\mu M^{\mu\alpha} \ , \tag{S3}$$

and the components of the normal stress vectors are

$$S^\alpha = -M^{\alpha\beta}_{;\beta} \ , \tag{S4}$$

where $b^\beta_\alpha = a^{\beta\lambda}b_{\lambda\alpha}$. The components of the stress vectors depends on the energy density as [1]

$$\Sigma^{\alpha\beta} = \rho\left(\frac{\partial F}{\partial a_{\alpha\beta}} + \frac{\partial F}{\partial a_{\beta\alpha}}\right) \text{ and } M^{\alpha\beta} = \frac{\rho}{2}\left(\frac{\partial F}{\partial b_{\alpha\beta}} + \frac{\partial F}{\partial b_{\beta\alpha}}\right) \ , \tag{S5}$$

where ρ is the surface mass density of the membrane. The tangential and normal local force balances can now be obtained by introducing Eqs. S2, S3, and S4 into Eq. S1, resulting in

$$T^{\beta\alpha}_{;\alpha} - S^\alpha b^\beta_\alpha = 0 \quad \text{and} \quad S^\alpha_{;\alpha} + T^{\beta\alpha}b_{\beta\alpha} + p = 0 \ , \tag{S6}$$

where we made use of the Gauss and Weingarten equations [2] $\mathbf{a}_{\alpha;\beta} = b_{\alpha\beta}\mathbf{n}$ and $\mathbf{n}_{,\alpha} = -b_{\alpha}^{\beta}\mathbf{a}_{\beta}$ respectively.

The free energy density can be written as a function of the mean curvature H and Gaussian curvature K. These are related to the metric and curvature by

$$H = \frac{1}{2}a^{\alpha\beta}b_{\alpha\beta} \quad \text{and} \quad K = \frac{1}{2}\varepsilon^{\alpha\beta}\varepsilon^{\lambda\mu}b_{\alpha\lambda}b_{\beta\mu} \ , \tag{S7}$$

where $a^{\alpha\beta} = (a_{\alpha\beta})^{-1}$ is the dual metric, and $\varepsilon^{\alpha\beta}$ is the permutation tensor defined by $\varepsilon^{12} = -\varepsilon^{21} = 1/\sqrt{a}$, $\varepsilon^{11} = \varepsilon^{22} = 0$. According to this definition (Eq. S7), the free energy density per unit mass can be re-written in terms of the mean and Gaussian curvatures $F(H, K; \theta^{\alpha})$. Furthermore, lipid membranes are essentially incompressible (see assumption (d) in the Model Development Section of the main text). This is imposed using a Lagrange multiplier $\gamma(\theta^{\alpha})$ to ensure that the local area dilatation $J = 1$, or equivalently, to constraint the constant surface density ρ of the membrane. Consequently we can define the surface energy density of the membrane as follows

$$F(\rho, H, K; \theta^{\alpha}) = \bar{F}(H, K; \theta^{\alpha}) - \frac{\gamma(\theta^{\alpha})}{\rho} \ , \tag{S8}$$

and when introducing the surface energy per unit area $W(\rho, H, K; \theta^{\alpha}) = \rho\bar{F}(H, K; \theta^{\alpha})$, the components of the stress vectors (Eqs. S5) can be written as [1]

$$\Sigma^{\alpha\beta} = (\lambda + W)a^{\alpha\beta} - (2HW_H + 2KW_K)\,a^{\alpha\beta} + W_H\tilde{b}^{\alpha\beta} \tag{S9}$$

$$M^{\alpha\beta} = \frac{1}{2}W_H a^{\alpha\beta} + W_K\tilde{b}^{\alpha\beta} \tag{S10}$$

where $\lambda(\theta^{\alpha}) = -\left[\gamma(\theta^{\alpha}) + W(H, K; \theta^{\alpha})\right]$, and $\tilde{b}^{\alpha\beta} = 2Ha^{\alpha\beta} - b^{\alpha\beta}$ is the cofactor of the curvature. The subscripts H and K refer to the partial derivative of the energy with respect to the indicated variable. Note that the Lagrange multiplier γ can be interpreted as a surface pressure, and is not a material property of the surface [3, 4]. Consequently, λ can be interpreted as the surface tension based on comparisons with edge conditions on a flat surface [4].

Finally, introducing Eqs. S9 and S10 into Eqs. S3 and S4, we can rewrite the normal and tangential force balances (Eqs. S6) as

$$\Delta\left(\frac{1}{2}W_H\right) + (W_K)_{;\alpha\beta}\tilde{b}^{\alpha\beta} + W_H(2H^2 - K) + 2H(KW_K - W) = p + 2\lambda H \ , \tag{S11}$$

and

$$-\left(\gamma_{,\alpha} + W_K K_{,\alpha} + W_H H_{,\alpha}\right)a^{\beta\alpha} = \left(\left.\frac{\partial W}{\partial\theta^{\alpha}}\right|_{\text{exp}} + \lambda_{,\alpha}\right)a^{\beta\alpha} = 0 \ , \tag{S12}$$

where $\Delta(\cdot) = (\cdot)_{;\alpha\beta}a^{\alpha\beta}$ is the surface Laplacian (or Beltrami operator), and $\partial(\cdot)/\partial\theta^{\alpha}\ |_{\text{exp}}$ is the explicit derivative with respect to θ^{α}.

Eqs. S11 and S12 are the general shape equation and incompressibility condition for an elastic surface with free energy per unit area $W(\rho, H, K; \theta^{\alpha})$.

S2 Helicoid to catenoid transformation

According to the Gauss' *Theorema Egregium*, the distribution of Gaussian curvature on a minimal surface follows any isometric mapping of such surface [5]. As illustrated in Fig. 2b, such transformation exists between helicoids and catenoids.

Elementary surface	Surface evolution sequence
P-Schwartz	g 5; r; g 5; r; g 5; r; g 10; u; r; g 10; u; r; g 10; u; u; refine edge where on_constraint 2; refine edge where on_constraint 4; hessian; hessian; u ;
D-Schwartz	g 5; r; g 5; r; g 5; r; g 10; u; r; g 10; u; r; g 10; u; u; hessian; hessian; r ; g 100; hessian; hessian ; g 100; u; g 500 ; hessian; g 100;

Table S1: Command sequence to refine the surface meshes of the elementary P- and D-Schwartz elementary surfaces. Description of the commands can be found in the Surface Evolver documentation.

Helicoids and catenoids belong to the same associated family of surfaces. The (continuous) isometric transformation from one surface to the other can be written as

$$\begin{cases} x = \sin(\alpha) r_n \cosh(u/r_n)\sin(\phi) - \cos(\alpha) r_n \sinh(u/r_n)\cos(\phi) \\ y = -\sin(\alpha) r_n \cosh(u/r_n)\cos(\phi) - \cos(\alpha) r_n \sinh(u/r_n)\sin(\phi) \\ z = \sin(\alpha) u + \cos(\alpha) r_n \phi \end{cases} \quad \text{with} \begin{cases} \phi \in [-\pi; \pi[\\ u \in [-H_c/2; H_c/2] \\ \alpha \in [0; \pi/2] \end{cases}, \tag{S13}$$

where P is the helicoid pitch, related to the catenoid neck radius by $r_n = P/(2\pi)$, and L is the helicoid diameter, related to the catenoid heigh by $H_c = 2r_n \sinh^{-1}(L/(2r_n))$.

For $\alpha = \pi/2$, this system describes a catenoid such as the one shown in Fig. 2c, while for $\alpha = 0$ it describes a helicoid as in Fig. 2a. The equivalence between Eqs. S13 and 7 when $\alpha = 0$ can be verified with the change of variable $r = r_n \sinh(u/r_n)$. Any intermediate values of α gives rise to a minimal surfaces belonging to the associated family of helicoids and catenoids, as illustrated in Fig. 2b.

The Gaussian curvature of these surfaces is given by

$$K = -\left(\frac{P/(2\pi)}{[P/(2\pi)]^2 + r^2}\right)^2 = -\left(\frac{r_n}{r_n^2 + [r_n \sinh(u/r_n)]^2}\right)^2. \tag{S14}$$

S3 Method for computing the distribution of spontaneous curvature on TPMS

Elementary surfaces P-Schwartz or D-Schwartz were downloaded from [1] and imported in Surface Evolver [6]. The surface energy was minimized through a succession of minimization and mesh refinement operations (see Table S1). The refined elementary surfaces were then duplicated and flipped to produce the periodic cubic unit cells, before to be exported in .stl format [2].

The cubic unit cell meshes were imported in Comosol Multiphysics, and Eq. 9 was solved using the "Surface reaction" module. Because of the periodic nature of the TPMS, instead of imposing Dirichlet boundary conditions at the boundaries, we chose periodic flux boundary conditions at the opposite edges, and imposed a surface average of C_0 on the unit cells. This choice is inspired from approaches to solve closure problems in transport in porous media, where the elementary unit volume is assumed to be periodic [7, 8].

References

[1] Steigmann DJ. Fluid Films with Curvature Elasticity. Archive for Rational Mechanics and Analysis. 1999 Dec;150(2):127–152. doi:10.1007/s002050050183.

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[1] `facstaff.susqu.edu/brakke/evolver/examples/periodic/periodic.html` (consulted on January 29th, 2019)
[2] `github.com/kashif/evolver/blob/master/fe/stl.cmd` (consulted on January 29th, 2019)

[3] Rangamani P, Agrawal A, Mandadapu KK, Oster G, Steigmann DJ. Interaction between Surface Shape and Intra-Surface Viscous Flow on Lipid Membranes. Biomechanics and Modeling in Mechanobiology. 2013 Aug;12(4):833–845. doi:10.1007/s10237-012-0447-y.

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S4 Supplementary Figures

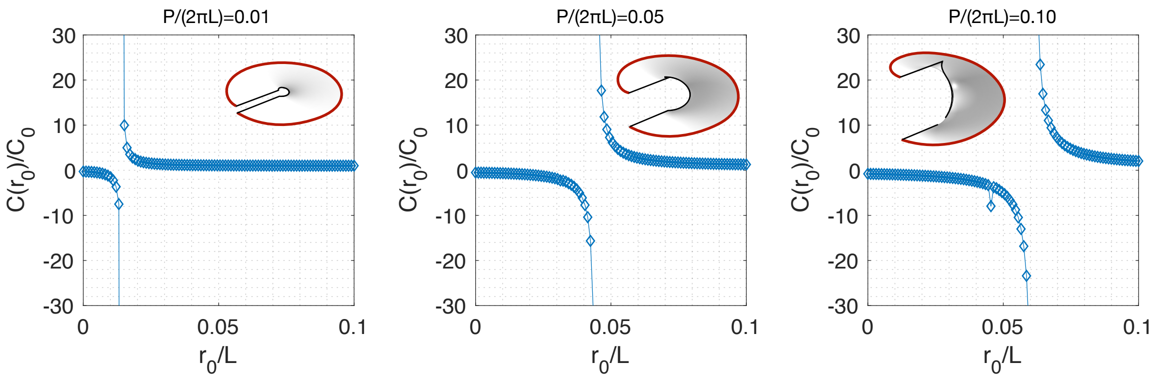

Figure S1: Helicoid pitch controls the position of the energy the spontaneous curvature switch in sign at the inner boundary.

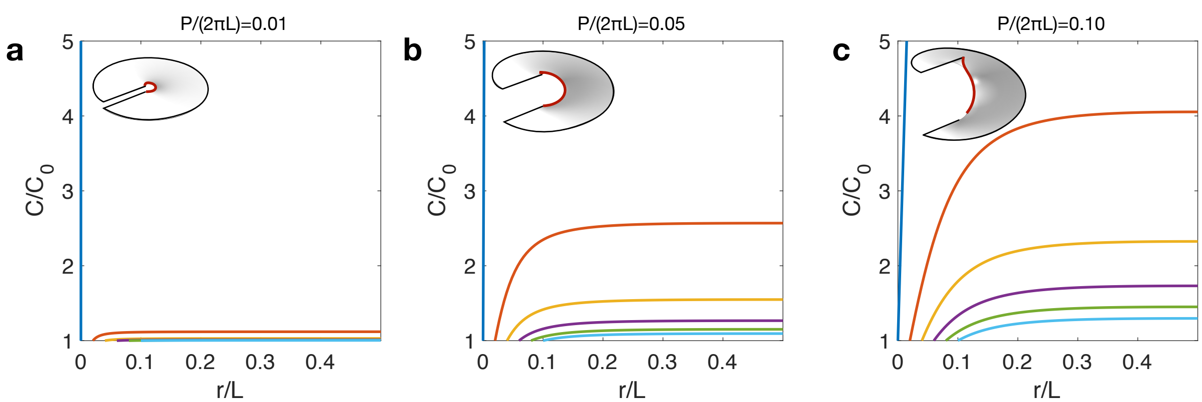

Figure S2: Distribution of spontaneous cutvature along the helicoid radius for C_0 imposed at the inner boundary of the catenoid for various pitch and inner radii. No switch is observed.

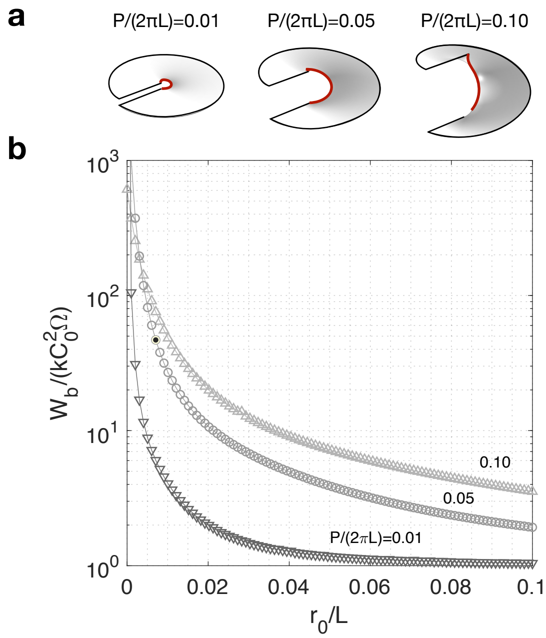

Figure S3: Normalized bending energy of helicoids with boundary conditions imposed on the inner bondary. No energy barrier is observed.

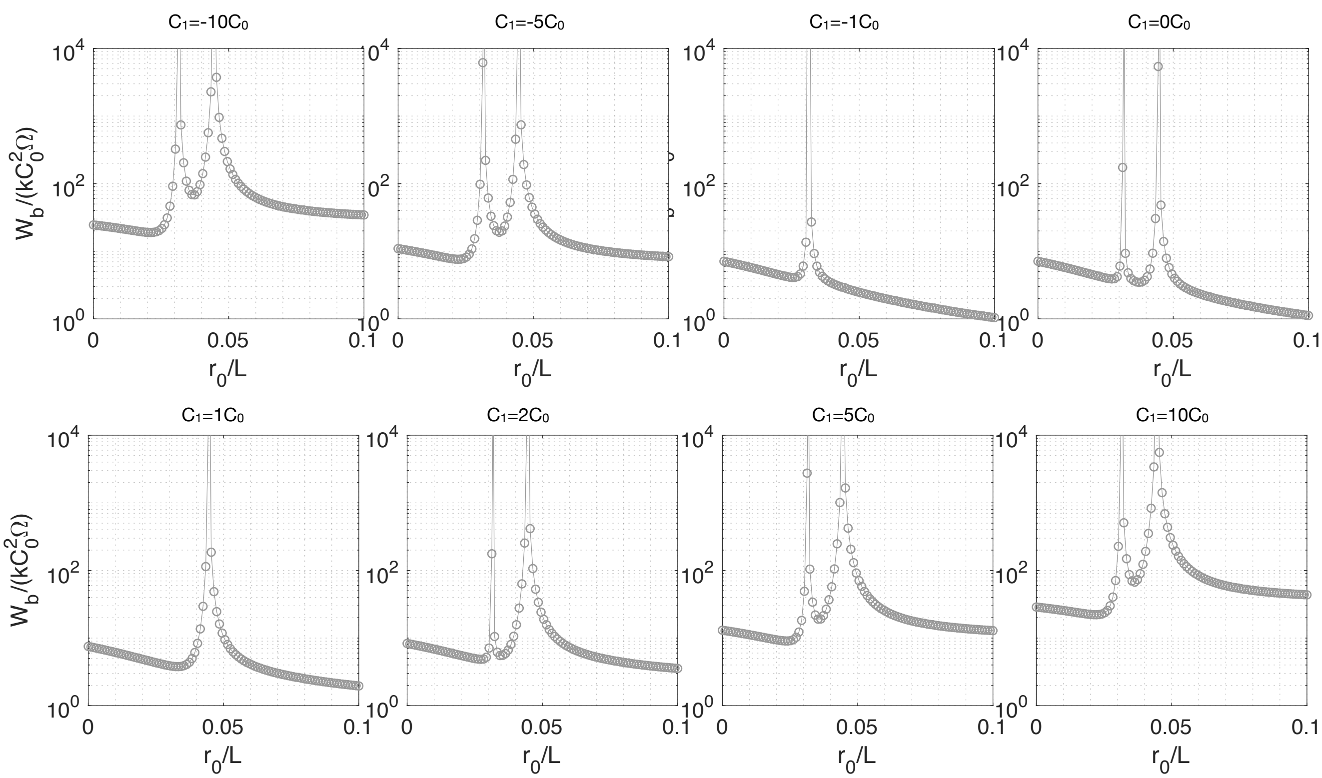

Figure S4: Effect of the imposed gradient in C at the external boundary on the bending energy of the helicoid.

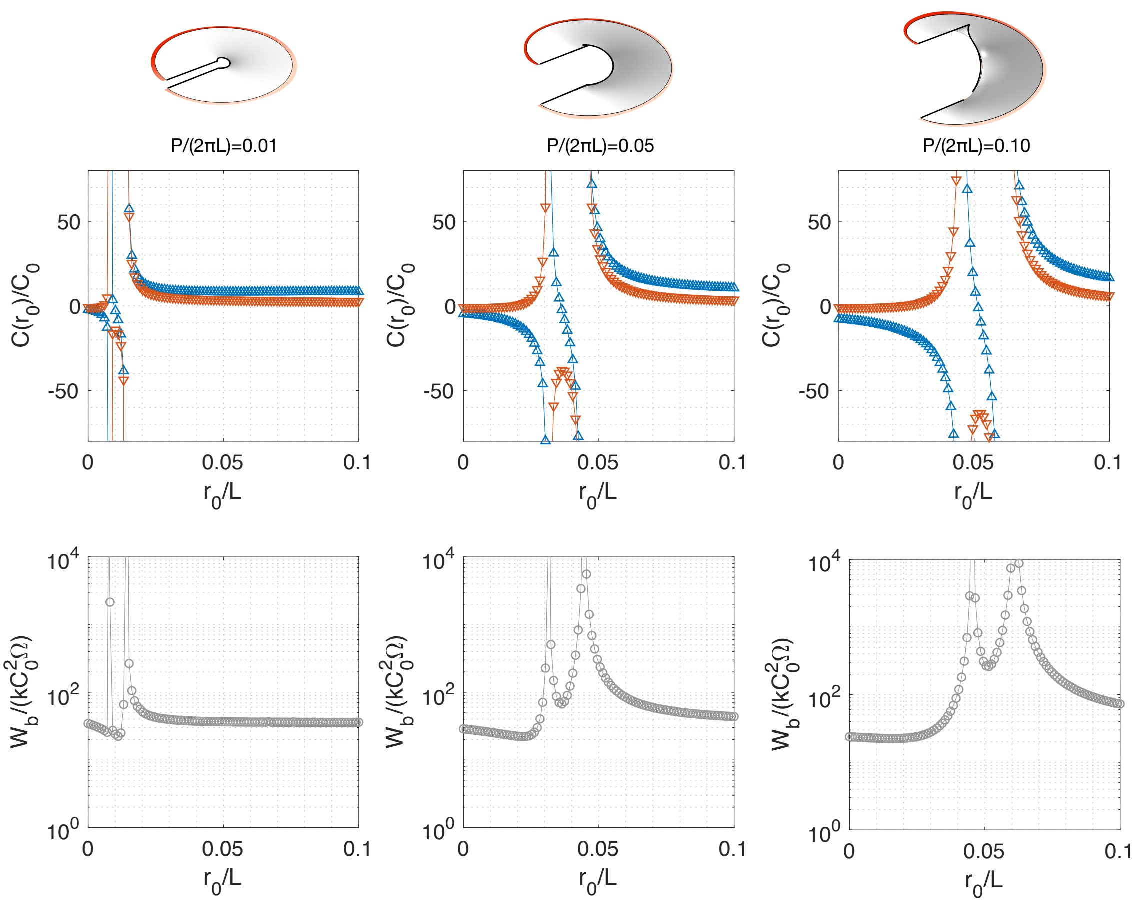

Figure S5: Effect of the pitch on the switch and energy barrier of helicoids with imposed gradient of boundary conditions at the exterior boundary.