Supplementary Information

Bactericidal mechanism of nanopatterned surface

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1. Free energy change of a bacterial cell during adhesion process on a cicada wing-like nanopatterned surface

When a bacterial cell is placed on a cicada wing-like nanopatterned surface, the bacterial cell can adhere to the patterned surface due to the larger adhesion energy than deformed bending energy and stretching energy of the membrane. Here we analyze the free energy change of the bacterial cell during adhesion process on cicada wing-like nanopatterned surface. The morphology of the cicada wing-like nanopatterned surface is defined by the a surface distribution density of ξ, the height of h, and the radius of R_p of nanopillars, as shown by Fig. S1 and described in the main text. The total free energy change of the system can be described as

$$\Delta E = \frac{1}{2}\lambda\frac{\Delta S^2}{S_0} + \left(E_{edge}^{Bend} + E_{ad}^{Bend} - E_0^{Bend}\right) - \gamma S_{ad} \tag{S1}$$

where λ is the stretching modulus of membrane, ΔS and S_0 are the area change and initial total area of bacterial cell membrane, E_{edge}^{Bend} is the deformed bending energy of the membrane at the edge of cell, E_{ad}^{Bend} is the bending energy of the deformed membrane at the bottom of the cell, E_0^{Bend} is the deformed bending energy of initial cell membrane, γ is the contact adhesion energy density between cell membrane and the patterned surface, and S_{ad} is the contact adhesion area.

In order to prove that the bacterial cell can be drawn by the patterned surface to adhere to the bottom of nanopillars in equilibrium, i.e. the nanopillars including their bottom can be completely adhered by cell membrane in the case of the nanopillars with the height of several hundred nanometers, we can analyze the free energy change with increasing adhesion depth H_a.

During the adhesion process, the membrane at the bottom of the cell is divided into three regions. The first is the contact adhesion region (region I) of the membrane with nanopillars. The second is the deformed region (region II) nearly contact adhesion region. The last is the undeformed region (region III) of the membrane. Figure S1(b) shows the schematic partially adhesion state of a nanopillar by the membrane. Therefore, the bending energy of the contact adhesion membrane E_{ad}^{Bend} in the second term of Eq. (S1) is divided into two parts: direct contact adhesion region and the deformed region nearly contact adhesion region (region II). So the bending energy of membrane adhered to a nanopillar can be calculated as $\left[4\pi\kappa+\pi\kappa\left(H_a-R_p-R'\right)/R_p+e_n\right]$, where $\left[4\pi\kappa+\pi\kappa\left(H_a-R_p-R'\right)/R_p\right]$ is the bending energy of the direct contact adhesion membrane, and e_n is the bending energy of the membrane in region II. e_n can be calculated by

$$
\begin{aligned}
e_n &= \int_{S_f}\left[\frac{\kappa}{2}\left(c_{f1}+c_{f2}-c_0\right)^2\right]d^2A \\
&= \int_0^{\pi/2}\left\{\frac{\kappa}{2}\left[\frac{1}{R'}+\frac{\sin\varphi}{R_p+R'-R'\sin\varphi}\right]^2 2\pi\left[R_p+R'-R'\sin\varphi\right]R'\right\}d\varphi \\
&= \pi\kappa\int_0^{\pi/2}\frac{\left(\frac{R_p}{R'}+1\right)^2}{\left(\frac{R_p}{R'}+1\right)-\sin\varphi}d\varphi
\end{aligned}
\tag{S2}
$$

Because $\left(\frac{R_p}{R'}+1\right)>1$, we have

$$e_n=\frac{2\pi\kappa\left(\frac{R_p}{R'}+1\right)^2}{\sqrt{\left(\frac{R_p}{R'}+1\right)^2-1}}\arctan\sqrt{\frac{\left(\frac{R_p}{R'}+1\right)+1}{\left(\frac{R_p}{R'}+1\right)-1}} \tag{S3}$$

According to Eq. (S3), we can find that the bending energy of membrane in region II is the function of R_p/R'. Therefore, we can obtain the equilibrium shape of the deformed membrane (R_p) by minimizing the bending energy. Fig. S2 shows the values of e_n as the function of R_p/R'. We can find that e_n has the minimum value of about 14.46κ when $R_p/R'\approx 0.599$. Therefore, the bending energy of membrane adhered to a nanopillar can be calculated as that $E_{ad}^{Bend}=\left[4\pi\kappa+\pi\kappa\left(H_a-R_p-R'\right)/R_p+14.46\kappa\right]\pi L^2\xi/4$.

The stretching free energy in the first term of Eq. (S1) can be calculated after knowing the change of the cell membrane area $\Delta S=S-S_0$. The total area of adhesion is that $S_{ad}=\left[2\pi R_p{}^2+2\pi R_p\left(H_a-R_p-R'\right)\right]\pi L^2\xi/4$, where $\pi L^2\xi/4$ represents the number of nanopillars adhered by membrane. The total area of membrane in the deformed region II can be calculated by $S_n=\left(\pi L^2\xi/4\right)\int_0^{\pi/2}2\pi\left[R_p+R'-R'\sin\varphi\right]R'd\varphi$, i.e. $S_n=\left(\pi^2L^2\xi R'/2\right)\left[\left(R_p+R'\right)\pi/2-R'\right]$. Therefore, we have that $S=\pi L^2/2+\pi^2LR+4\pi R^2+S_{ad}+S_n-\pi\left(R_p+R'\right)^2\left(\pi L^2\xi/4\right)$, and $\Delta S=S-S_0$.

The adhesion energy between the patterned surface and the cell membrane in the third term of Eq. (S1) can be calculated after knowing that $S_{ad}=\left[2\pi R_p{}^2+2\pi R_p\left(H_a-R_p-R'\right)\right]\pi L^2\xi/4$.

The dimensions of adhered cell (R and L) are associated with its volume. The

sunken volume caused by the adhesion with a nanopillar is that $V_{ad} = 2\pi R_p^3/3 + \pi R_p^2\left(H_a - R_p - R'\right) + v_n$, where v_n is sunken volume in the deformed region II, and $v_n = \pi R'\left[\frac{2}{3}R'^2 - \frac{\pi}{2}R'\left(R_p + R'\right) + \left(R_p + R'\right)^2\right]$ according to $v_n = \int_0^{\pi/2} \pi\left[R_p + R' - R'\sin\varphi\right]^2 R'\sin\varphi d\varphi$. So the total volume of the adhered cell can be given by $V = \pi L^2 R/2 + 4\pi R^3/3 + \pi^2 L R^2/2 - V_{ad}\,\pi L^2\xi/4$. According to the conservation of cell volume, we have the relation between R and L as

$$L = \frac{\sqrt{\left(\pi^2 R^2/2\right)^2 + \left(2\pi R - \pi\xi V_{ad}\right)\left(V_0 - 4\pi R^3/3\right)} - \pi^2 R^2/2}{2\left(\pi R/2 - \pi\xi V_{ad}/4\right)} \tag{S4}$$

Combining Eqs. (S1)-(S4), we can calculate the total free energy change of a bacterial cell adhered to a nanopatterned surface as the function of R and find the equilibrium stage of the cell by minimizing the total free energy change. In our calculation, $R_0 = 1\mu m$, $\lambda = 0.25 k_B T/nm^2$, $\kappa = 10 k_B T$, $\gamma = 0.1 k_B T/nm^2$, $\xi = 100\mu m^{-2}$, and $R_p = 40nm$. Fig. S3 shows the calculated free energy change as the function of radius of cell (R) under different adhesion depth, line (a) $H_a = 100nm$, line (b) $H_a = 200nm$, line (c) $H_a = 300nm$, line (d) $H_a = 400nm$, line (e) $H_a = 600nm$, line (f) $H_a = 800nm$, and line (g) $H_a = 1000nm$. We can find that the minimum free energy decreases with the increase of adhesion depth H_a, which means that the larger adhesion depth corresponds to the lower free energy, and the adhesion of cell can proceed favorably with the increase of adhesion depth. Therefore, when the height of nanopillars is several hundred nanometers, the bacterial cell can be drawn by patterned surface to adhere to the bottom of nanopillars in equilibrium. In other words, the nanopillars including their bottom can be completely adhered by cell membrane.

2. The bending energy change of the cell membrane on a flat substrate

As shown in Fig. (S4), the bending energy change of the cell membrane on a flat substrate can be given by the well known Canham-Helfrich Hamiltonian

$$E_{edge}^{Bend} = \int_{S_{edge}} \left[\frac{\kappa}{2} (c_1 + c_2 - c_0)^2 \right] d^2 A$$

$$= \int_0^{\pi} \left[\frac{\kappa}{2} \left(\frac{1}{R} + \frac{1}{R + \frac{L}{2\sin\theta}} \right)^2 \right] 2\pi \left(\frac{L}{2} + R\sin\theta \right) R d\theta$$

$$= \pi\kappa \int_0^{\pi} \left(4\sin\theta + \frac{\frac{L^2}{4R}}{R\sin\theta + \frac{L}{2}} \right) d\theta$$

Where κ is bending modulus of the membrane, c_1 and c_2 are two principal curvatures of the bending membrane surface, c_0 is the spontaneous curvature which is neglected in our model due to the large size of cell. The membrane surface at the edge of cell has two different principal curvatures. The first is the curvature of the vertical cross section of membrane $c_1 = 1/R$, and the other is the curvature of c_2. c_2 is determined by the location on the membrane surface. Because the curvature radius is equal to $[R + L/(2\sin\theta)]$ (as shown in the Fig. (S4)), we can obtain that $c_2 = [R + L/(2\sin\theta)]^{-1}$, where θ is the angle between vertical line on unreformed membrane surface and the line joining the center of the vertical cross section of edge membrane and local location on the deformed membrane surface, as shown in Fig. (S4).

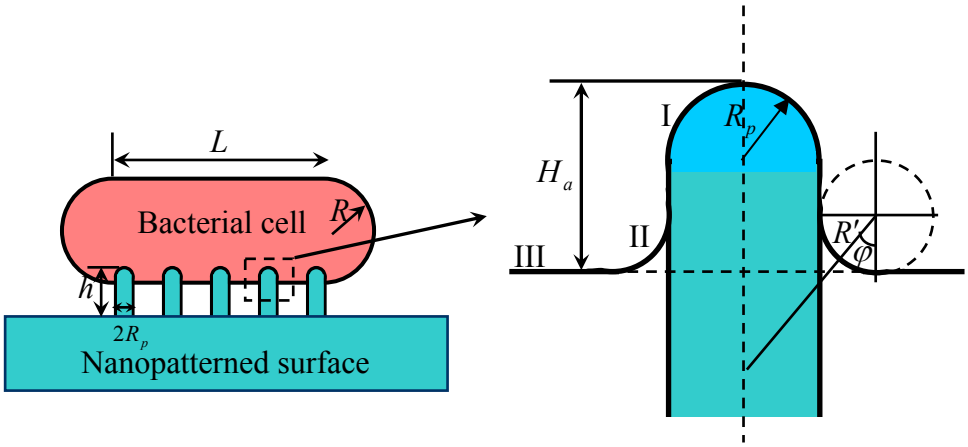

Fig. S1. Schematic illustration of a bacterial cell adhered to a cicada wing-like nanopatterned surface.

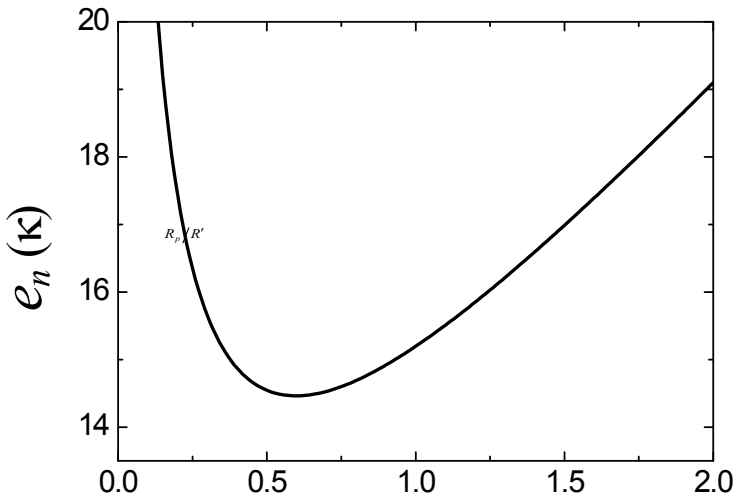

Fig. S2. The calculated values of e_n as the function of R_p/R' using Eq. (S3).

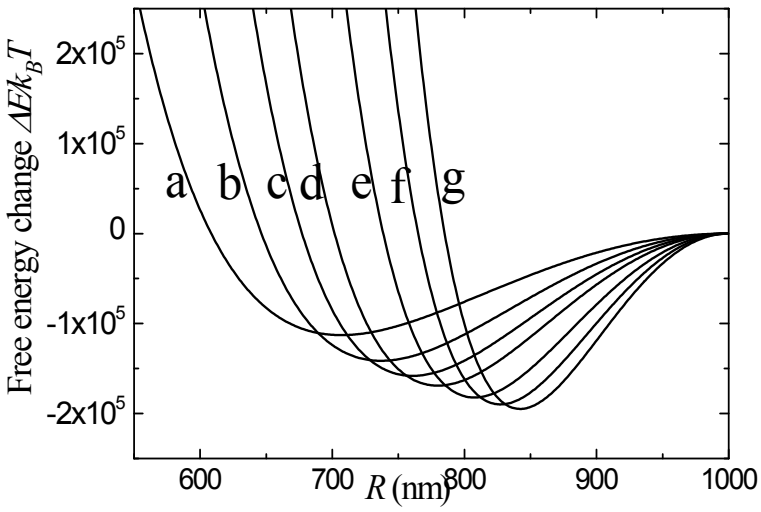

Fig. S3. The calculated free energy change as the function of radius of cell (R) under different adhesion depth, line (a) $H_a = 100nm$, line (b) $H_a = 200nm$, line (c) $H_a = 300nm$, line (d) $H_a = 400nm$, line (e) $H_a = 600nm$, line (f) $H_a = 800nm$, and line (g) $H_a = 1000nm$.

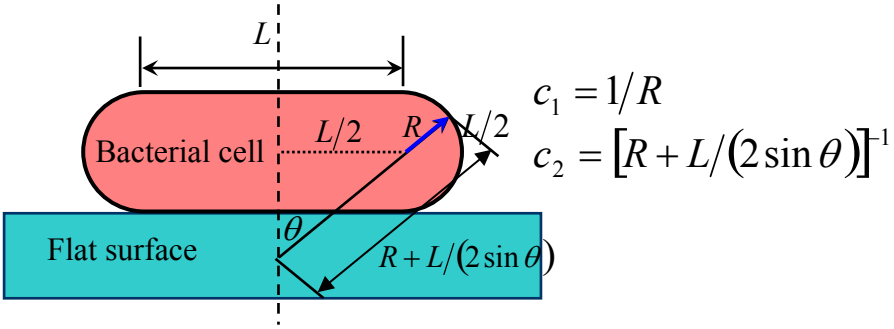

Fig. S4. The schematic illustration of the bacterial cell adhered to a flat surface.