Supporting Information for:

Adhesion and bending rigidity-mediated wrapping of carbon nanotubes by substrate-supported cell membrane

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1. Adhesion energy calculation

Because the system investigated here is two-dimensional, to calculate the integration over the arc length, the interaction between two infinite lines should be derived. Integrating the LJ potential along the infinite line, the cohesive energy per length between two parallel lines with distance h can be expressed as[1],

$$\Phi_1(h) = \frac{3\pi\varepsilon_{cm}\rho_m\rho_c\sigma_{cm}}{64}\left[21\left(\frac{\sigma_{cm}}{h}\right)^{11} - 32\left(\frac{\sigma_{cm}}{h}\right)^{5}\right], \tag{S1}$$

The adhesion strength between two surfaces is usually characterized by the adhesion energy per area U_{cm}. The relations between U_{cm} and ρ_m, ρ_c and ε_{cm} can be derived as follows. The van der Waals interaction energy between an area element dA and an infinite sheet is $\rho_m dA\int_0^x V(r)\rho_c 2\pi x dx$, so the adhesive energy per area between an area element and an infinite sheet is[2, 3]

$$\Phi_2(h) = \frac{\rho_m dA\int_0^x V(r)\rho_c 2\pi x dx}{dA} = 4\pi\varepsilon_{cm}\rho_m\rho_c{\sigma_{cm}}^6\left(\frac{{\sigma_{cm}}^6}{5h^{10}} - \frac{1}{2h^4}\right). \tag{S2}$$

The equilibrium separation distance can be determined by $\partial\Phi_2/\partial h = 0$, which leads to $h = \sigma_{cm}$. So the adhesion energy in equilibrium is $U_{cm} = -\Phi_2(\sigma_{cm}) = \frac{6}{5}\pi\varepsilon_{cm}\rho_m\rho_c{\sigma_{cm}}^2$. Then Φ_1 and Φ_2 can be expressed

$$\Phi_1(h) = \frac{5U_{cm}}{128\sigma_{cm}}\left[21\left(\frac{\sigma_{cm}}{h}\right)^{11} - 32\left(\frac{\sigma_{cm}}{h}\right)^{5}\right], \tag{S3}$$

$$\Phi_2(h) = \frac{10U_{cm}}{3}\left[\frac{1}{5}\left(\frac{\sigma_{cm}}{h}\right)^{10} - \frac{1}{2}\left(\frac{\sigma_{cm}}{h}\right)^{4}\right]. \tag{S4}$$

Combining Eqs. (4) and (S3), the adhesion energy between CNT and the membrane can finally be expressed as

$$E_{cm} = \iint \frac{5U_{cm}}{128\sigma_{cm}}\left[21\left(\frac{\sigma_{cm}}{h}\right)^{11} - 32\left(\frac{\sigma_{cm}}{h}\right)^{5}\right]ds_c ds_m. \quad \text{(S5)}$$

2. Energy diagrams

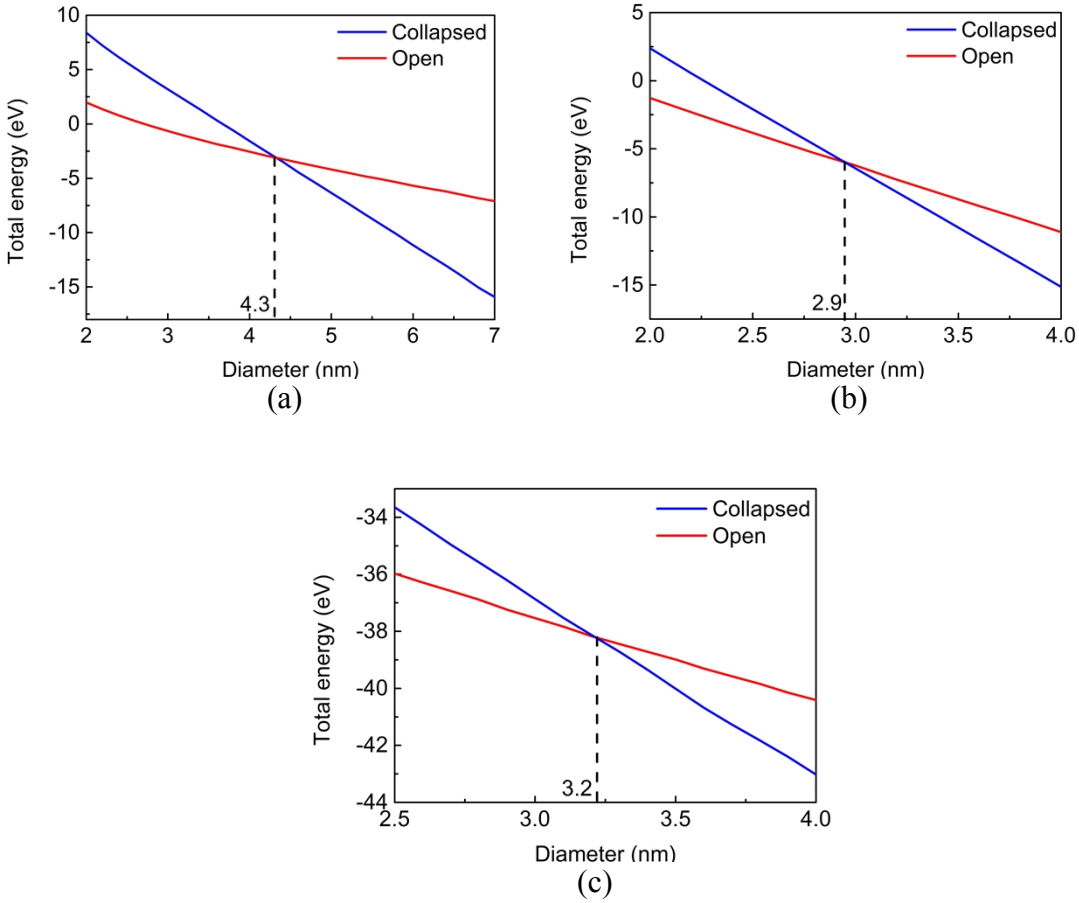


Fig. S1. Energy diagrams of systems with open (red lines) and collapsed (blue lines) CNTs: (a) free CNTs, (b) CNTs on a substrate and (c) CNT-membrane-substrate system. ($D_m = 4.0$ eV, $U_{cm} = 0.64$ eV/nm^2, $\sigma = 2 \times 10^{-3}$ eV/nm^2).

3. Transition between the neighbor minima.

To explore the transition between the neighbor minima, we used the nudged elastic band (NEB) algorithm to determine the energy barrier and minimum energy path of the transition. For CNT with $d = 3.5\ nm$ covered by membrane with $D_m = 4.0\ eV$ and $U_{cm} = 0.64\ eV/nm^2$, the collapsed configuration is more energetic stable than the open configuration and the energy difference is about $1.00\ eV/nm$. **Fig. S2** shows the results of the NEB calculations. The transition state occurs late along the path and the energy barrier is about $3.65\ eV/nm$ from the open configuration to the collapsed one.

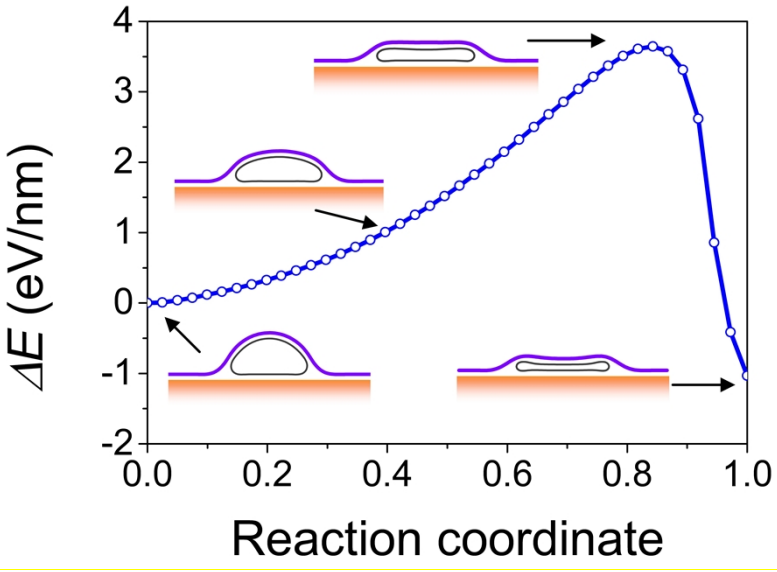


Fig. S2. The minimum energy path for the collapse of CNT covered substrate-supported membrane ($D_m = 4.0$ eV, $U_{cm} = 0.64$ eV/nm^2, $d = 3.5\ nm$). The zero of energy is relative to the open configuration and the energies are per unit length. The insets are configurations along the minimum energy path.

4. Approximate expression of the phase boundary in Fig. 6

In this section, simple modes are employed to give approximate expression of the phase boundary in Fig. 6. For the open configuration, the configuration of CNT is modeled by a semicircle with radius of R, which satisfies the relationship $\pi R + 2R = \pi d$. The bending energy of the CNT and membrane are $E_{bc} = \frac{D_c}{2}\left(\frac{1}{R}\right)^2 \pi R = \frac{D_c \pi}{2R}$ and $E_{bm} = \frac{D_m}{2}\left(\frac{1}{R+h}\right)^2 \pi (R+h) = \frac{D_m \pi}{2(R+h)}$, respectively. The CNT-membrane interaction energy is $E_{cm} = -\pi R U_{cm}$ and the CNT-substrate interaction energy is $E_{sc} = -2RU_{sc}$. The membrane-substrate interaction energy is $E_{sm} = -(2L - 2R - 2h)U_{sm}$. For the collapsed configuration, the bending energy of the CNT is mainly localized at the two highly strained ends, which can be modeled by two semicircles with radius of h, yielding $E_{bc} = \frac{D_c}{2}\left(\frac{1}{h}\right)^2 2\pi h = \frac{D_c 2\pi}{2h}$. The van der Walls self-interaction of the CNT is approximated by $E_{cc} = -\frac{1}{2}\pi d U_{cc}$. The membrane adopts a flatten configuration and its bending energy can be neglected in this simple model. Similar with the open configuration, the CNT-membrane and CNT-substrate are $E_{cm} = -\frac{1}{2}\pi d U_{cm}$ and $E_{sc} = -\frac{1}{2}\pi d U_{sc}$, respectively. The membrane-substrate interaction energy is $E_{sm} = -(2L - \frac{1}{2}\pi d - \alpha h)U_{sm}$, where α is an adjustment factor to consider the excessive length of the membrane detaching from the substrate as compared with the contact length between the CNT and the substrate, and here the adjustment factor equals approximately to 3 for the considered system. By equating the total energy of the open and collapsed configurations, U_{cm} can be expressed by D_m as

$$U_{cm} = \frac{2}{2R - d}\left[\frac{D_m}{2(R+h)} - \frac{D_c}{2}\left(\frac{2}{h} - \frac{1}{R}\right) + \frac{d}{2}U_{cc} + \left(\frac{d}{2} - \frac{2R}{\pi}\right)(U_{sc} - U_{sm}) - \frac{h}{\pi}U_{sm}\right]. \quad \text{(S6)}$$

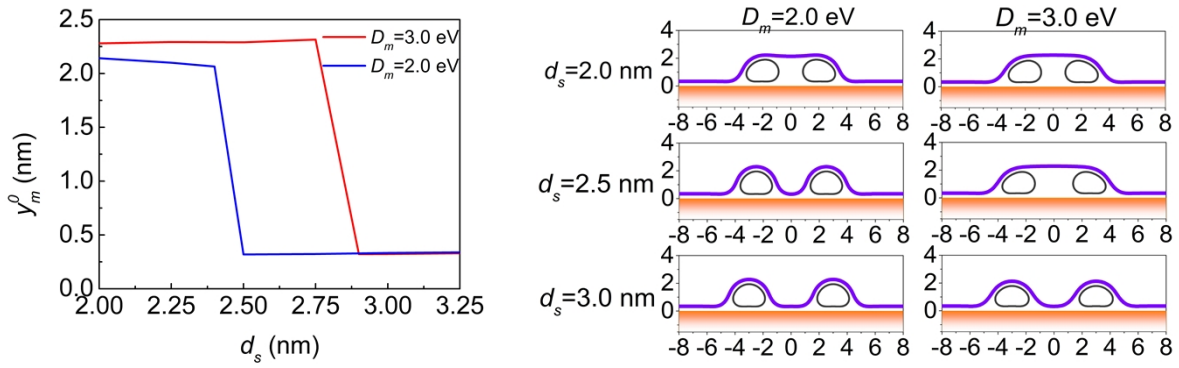
Let $d = 3.5\ nm$, $U_{sc} = U_{sm} = U_{cc} = 2.29\ eV/nm^2$ and $h = 0.34\ nm$, the phase boundary in Fig. 6 can be approximated by

$$U_{cm} = 0.519D_m - 0.079. \tag{S7}$$

The line is plotted in Fig. 6, which turns to be consistent with our calculation.

5. Configuration regulated by the distance between two CNTs

Besides the bending stiffness of the membrane, the morphology of the system can also be regulated by the center distance between the CNTs. The results for the systems with d_s varying from $2.00\ nm$ to $3.25\ nm$ are plotted in Fig. S3a. When the spacing between the CNTs is small, the membrane remains nearly flat and doesn't adhere to the substrate. In these cases, $y_m^0 = 2.10$ nm when $D_m = 3.0$ eV and $y_m^0 = 2.30$ nm when $D_m = 2.0$ eV, respectively. This is due to that the energy reduced by conforming to the CNTs and adhering to the substrate doesn't compensate the cost of membrane bending. On the other hand, when the spacing between two CNTs is large, the membrane will conform to the CNT and adhere to the substrate to gain the adhesion energy. In this case, y_m^0 is equal to the equilibrium distance between the membrane and the substrate. Similar to the case with various D_m, snap-through instability is also observed here. That is, for $D_m = 2.0$ eV when d_s slightly increases from $2.40\ nm$ to $2.50\ nm$, the membrane morphology between two CNTs sharply switches from adhering to the substrate to detaching from the substrate. When D_m increases to $3.0\ eV$, the critical spacing d_c^{cr} increases to about $2.80\ nm$, implying that larger spacing is needed for stiffer membrane to conform to the CNTs. Typical configurations with various CNTs spacings are shown in Fig. S3b.



(a) (b)

Fig. S3. (a) y_m^0 as a function of d_s when $D_m = 2.0$ eV (blue line) and $D_m = 3.0$ eV (red line). (b) Morphologies of the systems for the CNTs spacing of $d_s = 2.0$ nm, $2.5\ nm$ and $3.0\ nm$, from top to bottom, respectively.

References

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2. T. Tang, A. Jagota and C.-Y. Hui, *J. Appl. Phys*., 2005, **97**, 074304.
3. L. Y. Jiang, Y. Huang, H. Jiang, G. Ravichandran, H. Gao, K. C. Hwang and B. Liu, *J. Mech. Phys. Solids*, 2006, **54**, 2436.