Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary information

Perturbation of Pulmonary Surfactant Monolayer by Single-Walled Carbon Nanotubes: A Molecular Dynamics Study

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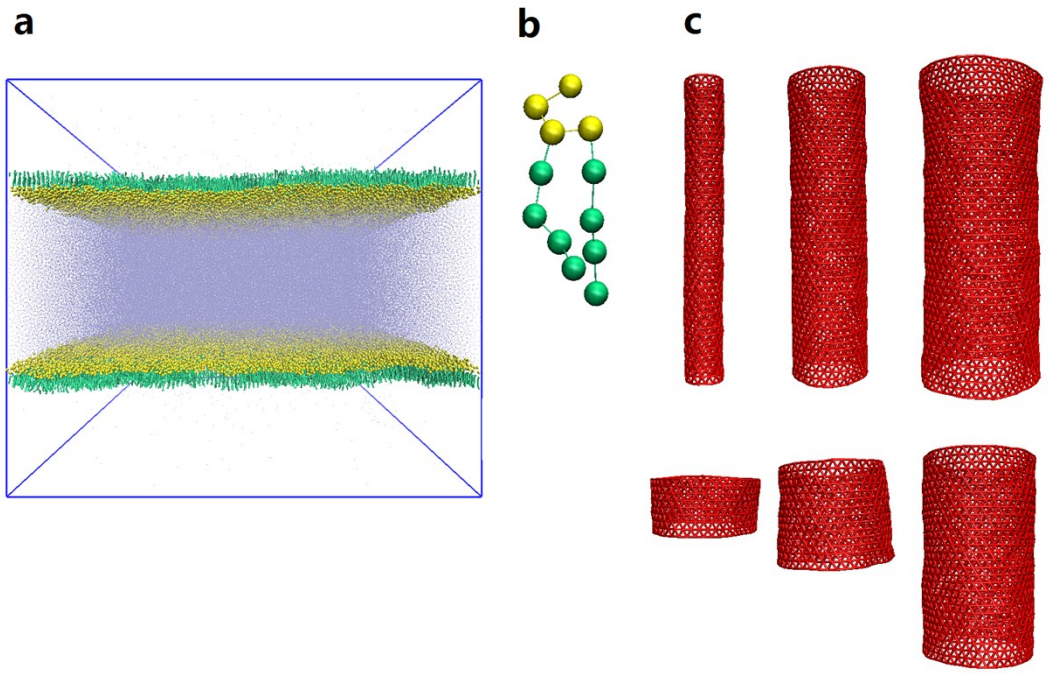

Fig. S1 Coarse-grained molecular dynamics simulation setup. (a) The initial configurations of the DPPC monolayer. (b) The coarse-grained DPPC model. (c) The coarse-grained model of SWCNTs with different sizes.

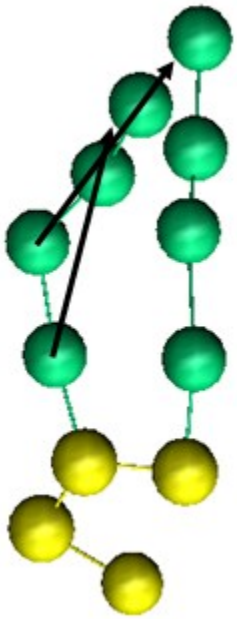

Fig. S2. CG model of a DPPC molecule to explain the calculation of the order parameter.

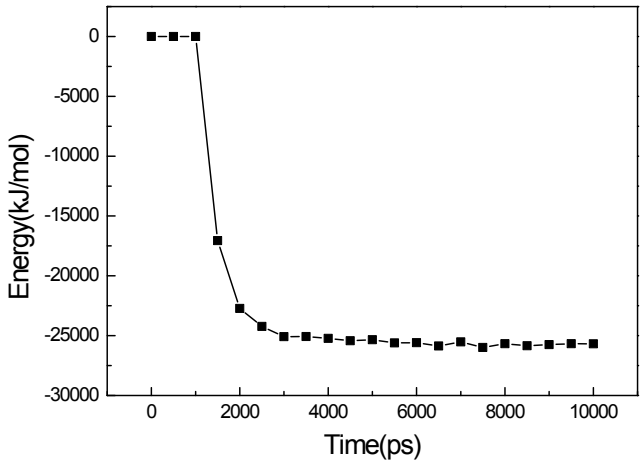

Fig. S3 Time evolution of interaction energy between SWCNT and lipids. The diameter and length of SWCNT are 5.28 nm and 4.47 nm, respectively.

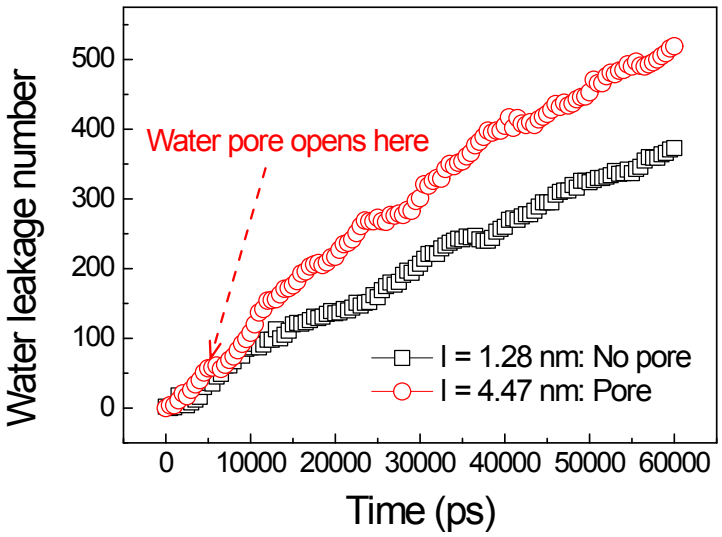

Fig. S4 Monitoring numbers of water molecules escaping from the monolayers inserted by an ultrashort SWCNT (l = 1.28 nm, black) and a short SWCNT (l = 4.47 nm, red).

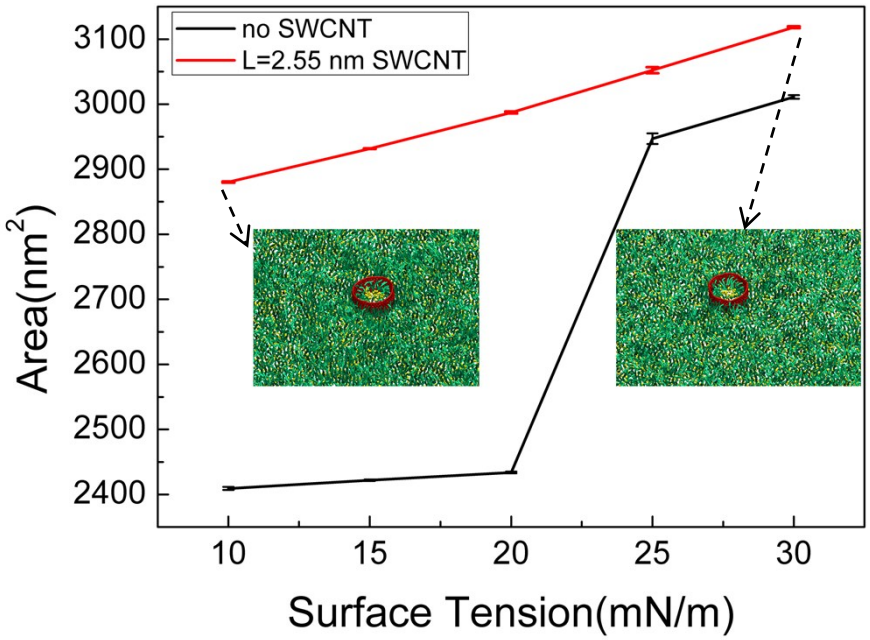

Fig. S5 The calculated monolayer area as a function of surface tension for both pure PSM and the PSM inserted by a short SWCNT with length of 2.55 nm.

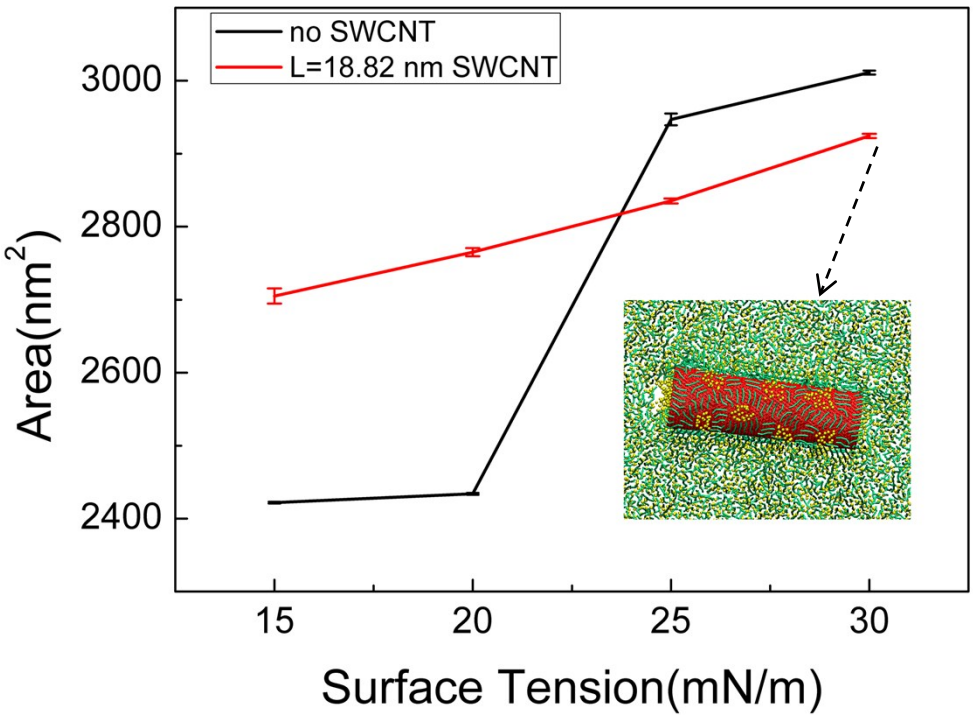

Fig. S6 The average monolayer area as a function of surface tension for both pure PSM and the PSM inserted by a SWCNT with length of 18.82 nm.

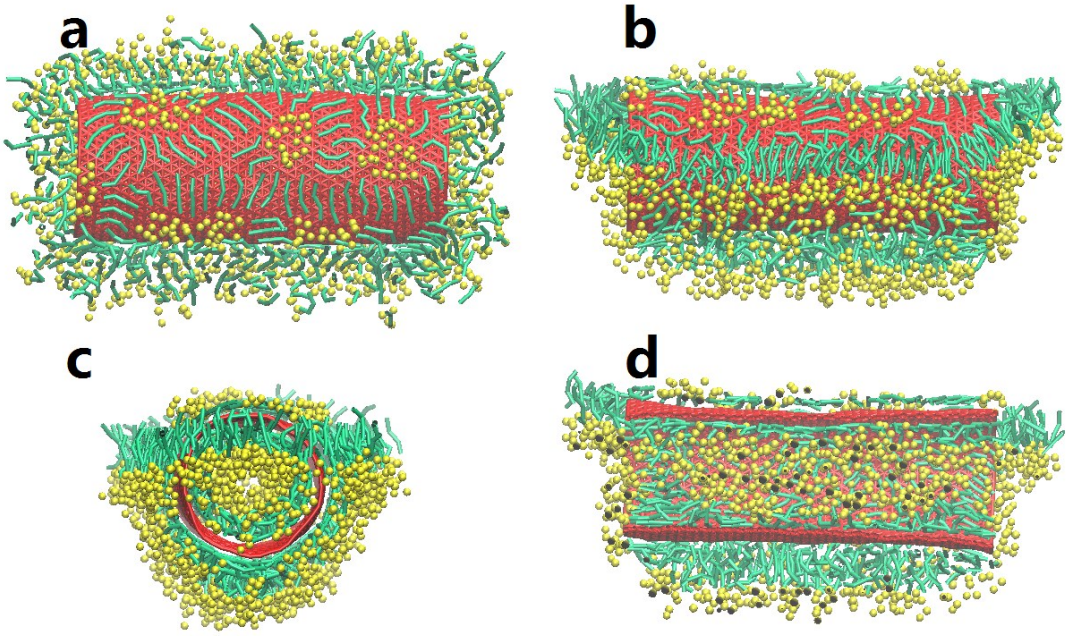

Fig. S7 Lipid arrangements around SWCNT with length of 14.04 nm and diameter of 5.28 nm. a) top view illustrating the inverse micelle assembly of lipids extracted from PSM; b) and c) side views illustrating the unperturbed lipids on PSM plane and semi-cylindrical micelle formation beneath the SWCNT; d) sectional view illustrating the lipid arrangement inside the tube.

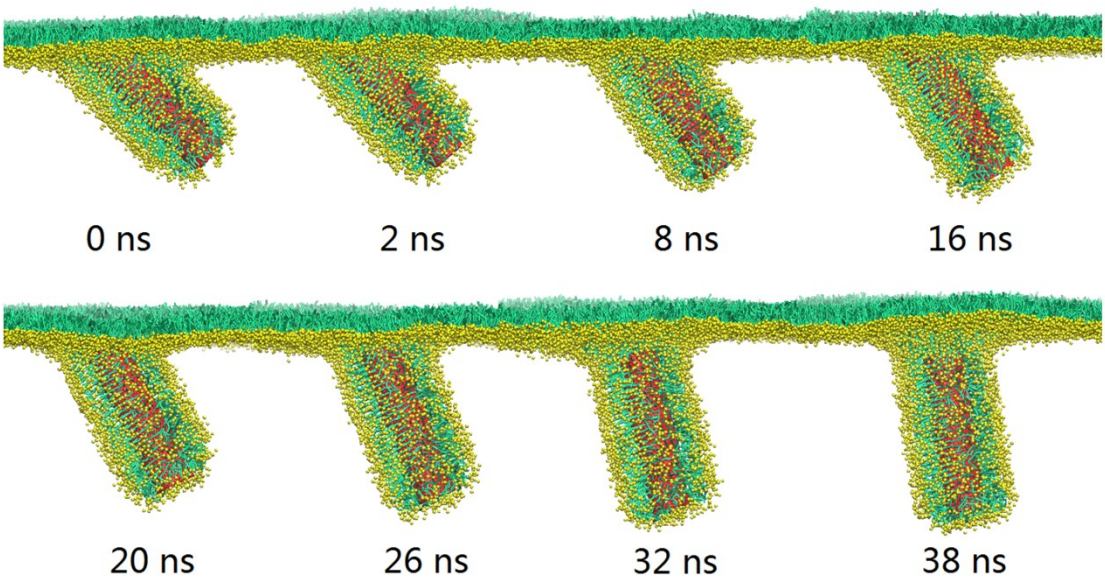

Fig. S8 Time sequence of MD simulation results showing a SWCNT with diameter of 3.52 nm and length of 14.04 nm interacting with PSM under surface tension of 10 mN m^{-1}. The fixed center of mass of SWCNT provides sufficient time for SWCNT to stand up. This result combines with unbiased simulation result in Figure 7 to verify that the final entry angle of SWCNT is a competition of time scales for tube rotation and PSM invagination.

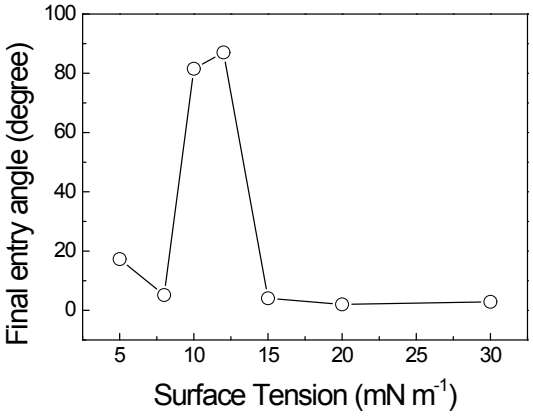

Fig. S9 The steady-state entry angle of SWCNT with a diameter of 5.28 nm and a length of 14.04 nm as a function of surface tension.

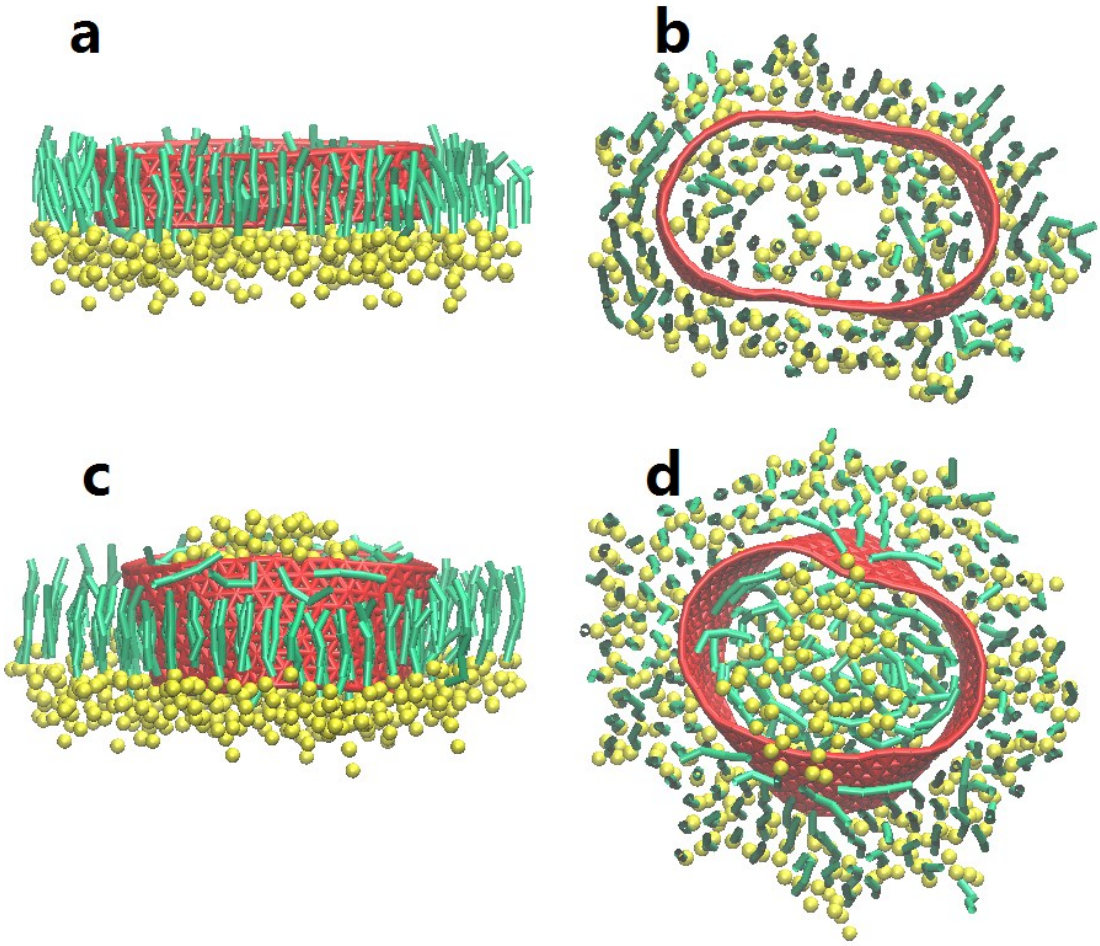

Fig. S10 Vertical insertion of short SWCNTs with slight perturbation under compression. a) and c) show the side views; b) and d) are the corresponding top views illustrating the lipid arrangement inside and above the tube. The tube diameter was set to 5.28 nm. The tube lengths are 1.28 nm (a and b), 2.55 nm (c and d).

Video captions:

Video S1. Insertion of a longer SWCNT into PSM with lipid extraction under expansion.

Video S2. Wrapping of a longer SWCNT by PSM with horizontal alignment via transforming monolayer into bilayer under compression.

Video S3. Vertical entry of SWCNT by increasing the tube diameter.

Video S4. Vertical entry of long SWCNT under external restraining force.

Video S5. PSM vesiculation to encapsulate short SWCNT.