Supplementary information

Surface Patterning of Single-Walled Carbon Nanotubes Enhances Their Perturbation on Pulmonary Surfactant Monolayer: Frustrated Translocation and Bilayer Vesiculation

Tongtao Yue,[a] Yan Xu,[a] Shixin Li,[a] Zhen Luo,[a] Xianren Zhang,[b] and Fang Huang[a]

[a]*State Key Laboratory of Heavy Oil Processing, Center for Bioengineering and Biotechnology, College of Chemical Engineering, China University of Petroleum (East China), Qingdao, 266580, China. E-mail: yuett@upc.edu.cn*
[b]*State Key Laboratory of Organic-Inorganic Composites, College of Chemical Engineering, Beijing University of Chemical Technology, Beijing, 100029, China.*
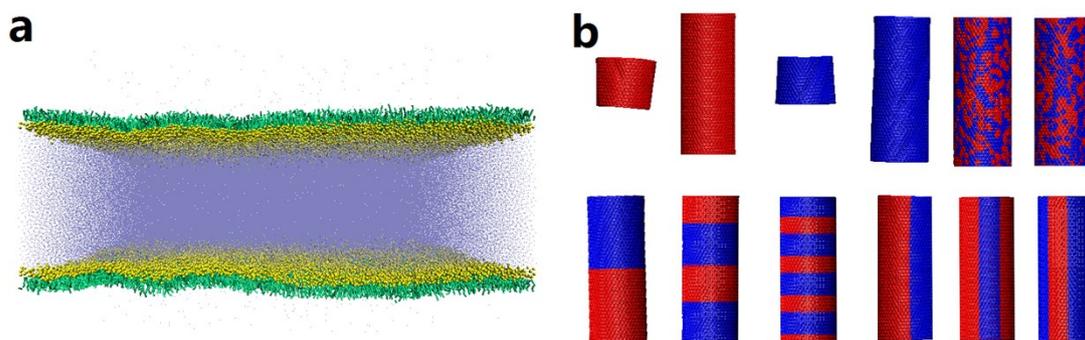
Fig. S1 Simulation system setup. (a) bi-monolayer PSM model; (b) coarse-grained model of pristine, hydrophilic, and surface patterned SWCNTs.
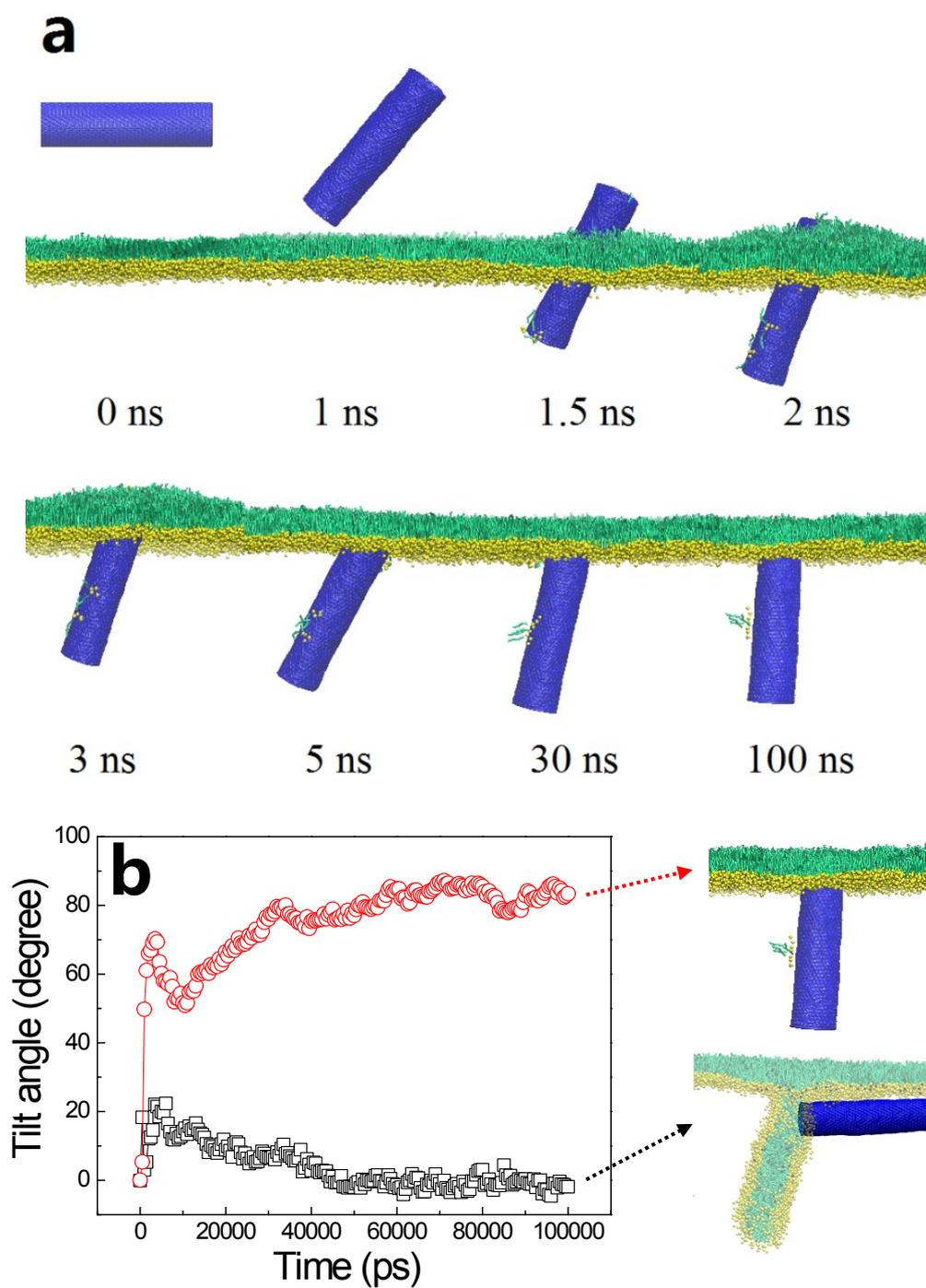
Fig. S2 Repeat MD simulation showing direct translocation of hydrophilic SWCNT with no PSM perturbation. (a) Typical snapshots, (b) Time evolutions of orientation angle of SWCNT in two independent simulations. The PSM tension was fixed to 10 mN m^{-1}.
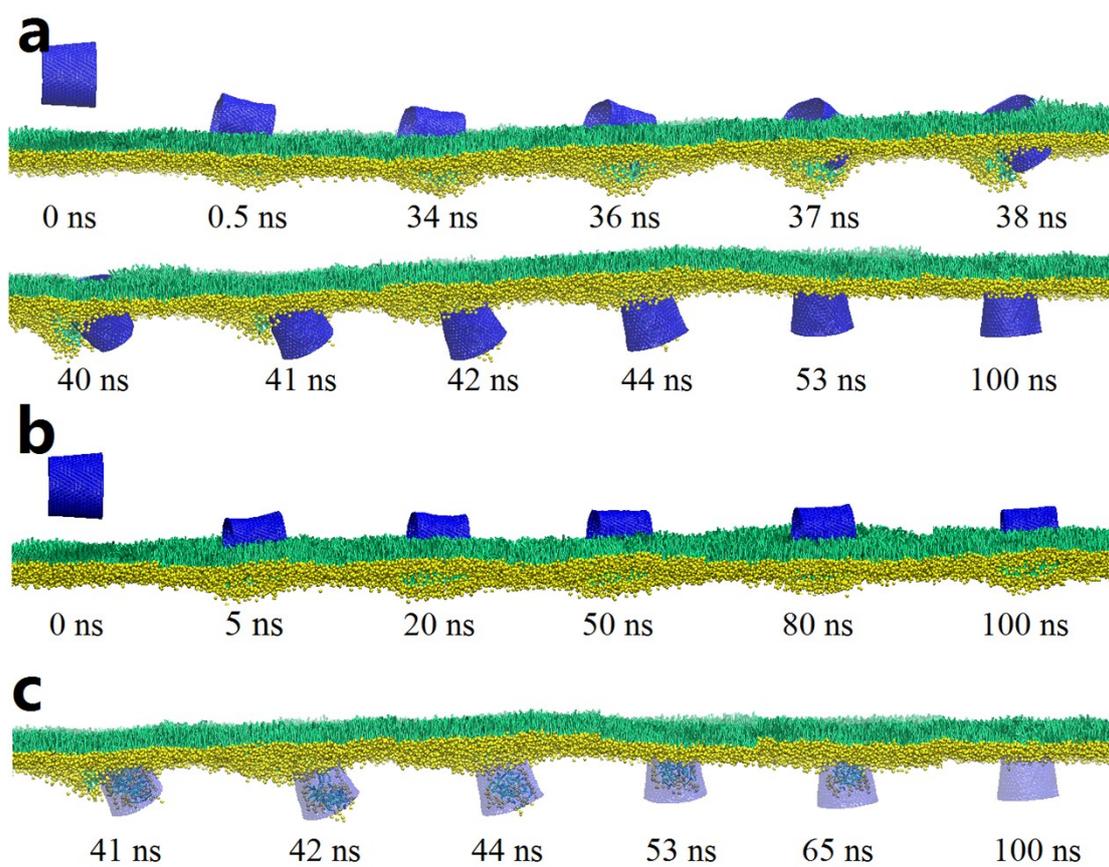
Fig. S3 Repeat simulations revealing distinct PSM interaction pathways of short hydrophilic SWCNT. (a) Direct translocation without PSM perturbation. (b) Failed translocation of SWCNT being trapped at the monolayer-air interface. (c) Lipid protrusion and subsequent recoverage inside the tube.
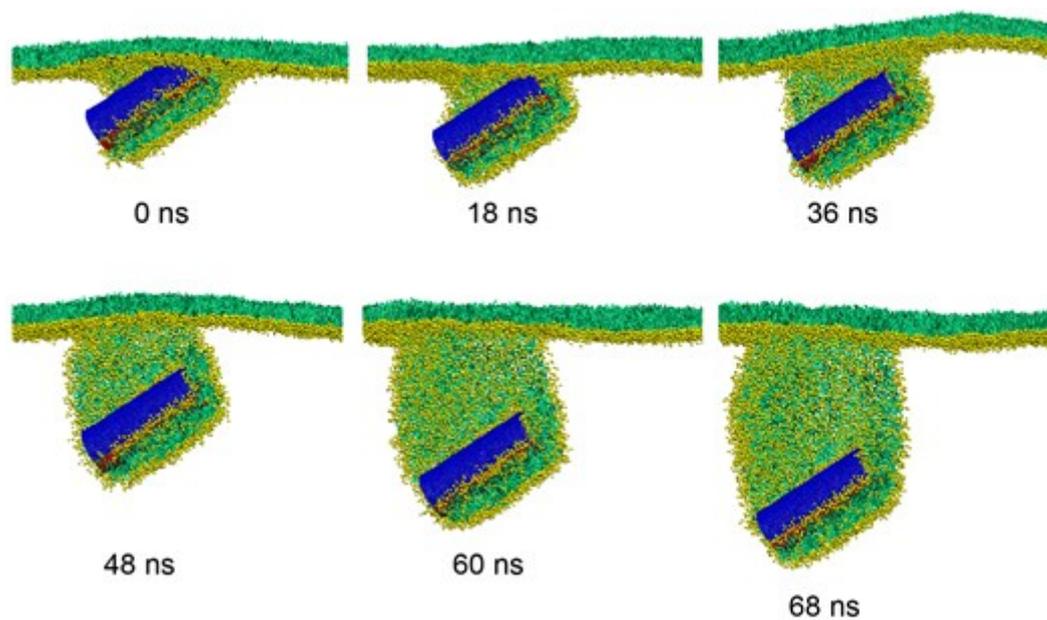
Fig. S4 Time sequence of MD simulation results showing a SWCNT with two axial stripes interacting with PSM under expiration. The SWCNT was fixed along x and y directions but free along z direction. This result combines with the unbiased simulation result in Figure 9 to verify the importance of self-rotation of SWCNT in PSM vesiculation.
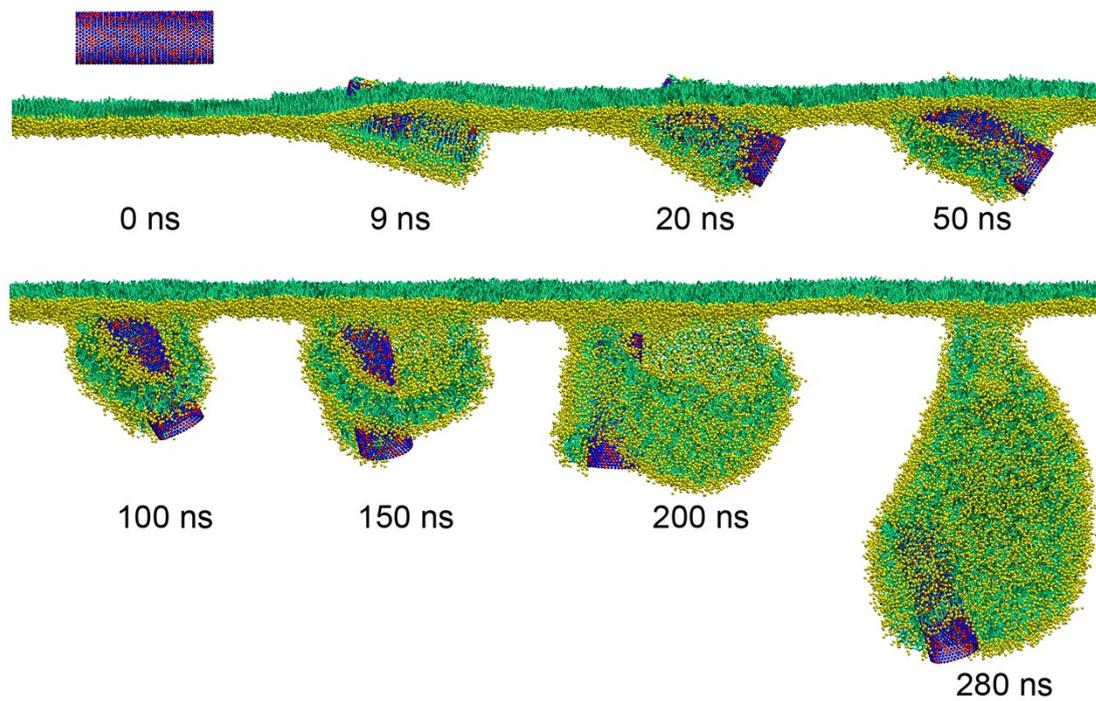
Fig. S5 Simulated PSM vesiculation event by interacting with random surface patterned SWCNT with hydrophobic ratio of 0.3.
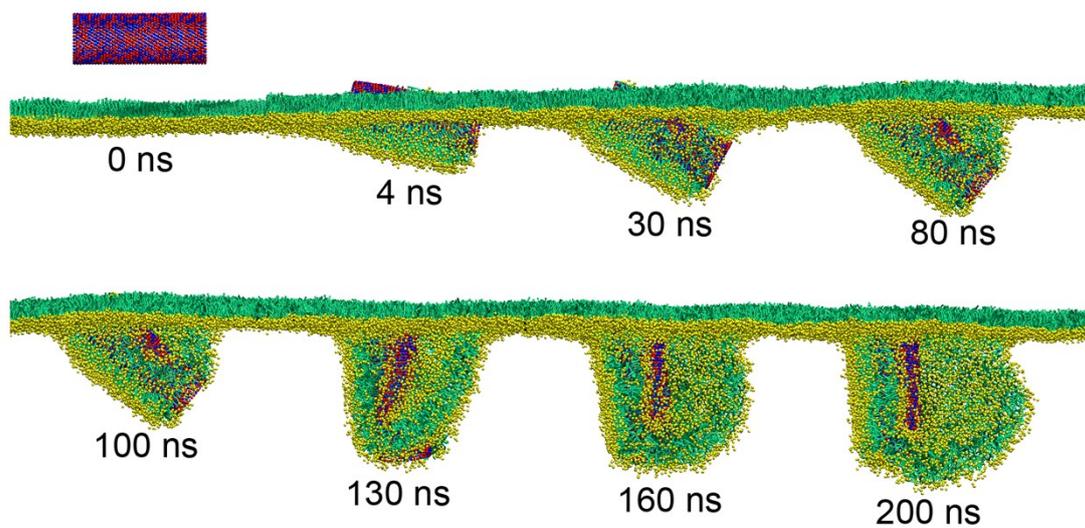
Fig. S6 Simulated semi-vesiculation event by interacting with random surface patterned SWCNT with hydrophobic ratio of 0.5.
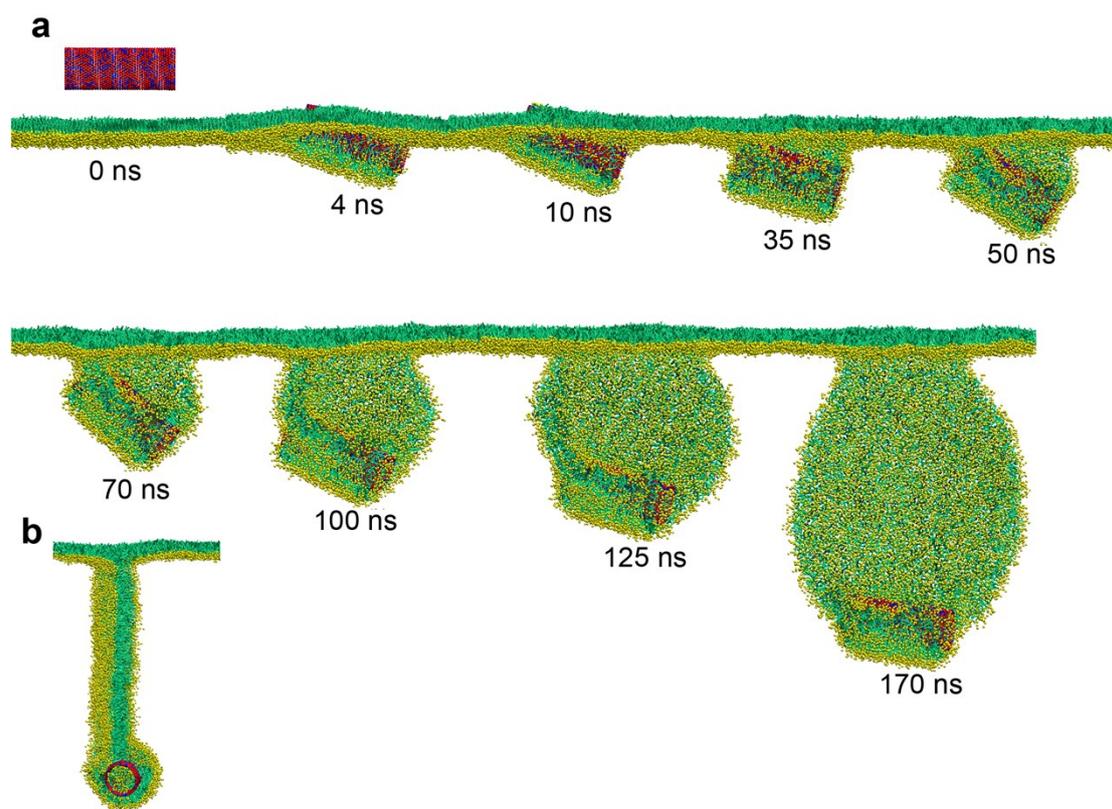
Fig. S7 Random patterned SWCNT with hydrophobic ratio of 0.7 behaves like pristine SWCNT and was wrapped by the PSM folding bilayer under compression. (a) Typical snapshots. (b) Cross sectional view of the final structure illustrating the detailed wrapping state.