Supplementary Information for

Manipulating Molecular Order in Nematic Liquid Crystal Capillary Bridges via Surfactant Adsorption: Guiding Principles from Dissipative Particle Dynamics Simulations

Zeynep Sumer and Alberto Striolo*

Department of Chemical Engineering, University College London

London WC1E 7JE, United Kingdom

Table S1. Repulsion coefficients (α) used in the simulations in k_BT units.

	Water	***LC***	***S_{head}***	***S_{tail}***
Water	25	50	25	50
LC		25	50	20, 25
S_{head}			25	50
S_{tail}				25

Table S2. Compositions of simulated systems with (a) 1000 surfactant molecules where $\alpha_{LC\text{-}Stail} = 25$; (b) 1500 surfactant molecules where $\alpha_{LC\text{-}Stail} = 25$; and (c) 1000 surfactant molecules where $\alpha_{LC\text{-}Stail} = 20$.

	Water	***LC***	***Surfactant***
a	65.43%	22.22%	12.35%
b	59.26%	22.22%	18.52%
c	65.43%	22.22%	12.35%

Table S3. Orientational order parameters (S) of LC molecules when different surfactants are adsorbed on the LC cylinder with S_{head}/S_{tail} = (a) 3/5, (b) 7/5, and (c) 5/7 at 0.7 k_BT. Data are shown as a function of distance from the cylindrical axis ($r_c = 0$). Values given in bold are the results discussed in the paper.

	Head Beads	***Tail Beads***	***S ($r \leq 5\ r_c$)***	***S ($r > 5\ r_c$)***	***$S_{overall}$***
	5	**5**	**0.57±0.05**	**0.43±0.03**	**0.49±0.03**
a*	3	5	0.53±0.05	0.37±0.04	0.44±0.03
b	7	5	0.54±0.05	0.41±0.03	0.46±0.03
	3	**7**	**0.53±0.05**	**0.27±0.04**	**0.38±0.04**
c	5	7	0.57±0.03	0.27±0.04	0.39±0.02

* Simulation was conducted for 0.894 μs, and the result is the outcome of last 0.149 μs. See narrative for relevant discussion on the simulation length.

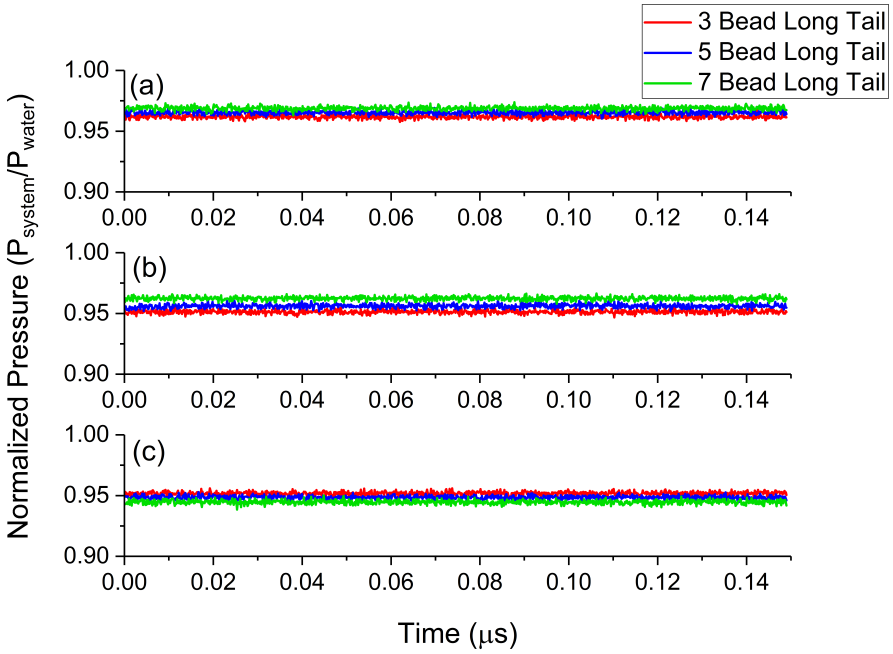

Figure S1. Normalized pressures of the systems with (a) 1000 surfactant molecules where $\alpha_{LC\text{-}Stail} = 25$; (b) 1500 surfactant molecules where $\alpha_{LC\text{-}Stail} = 25$; and (c) 1000 surfactant molecules where $\alpha_{LC\text{-}Stail} = 20$. The legend is the same for (a), (b) and (c).

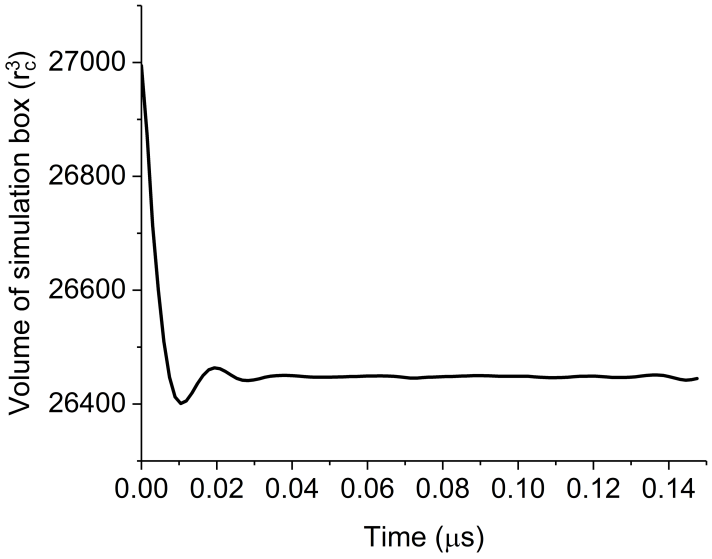

Figure S2. Volume change of the system that was simulated for additional 0.14 μs in NPT ensemble.

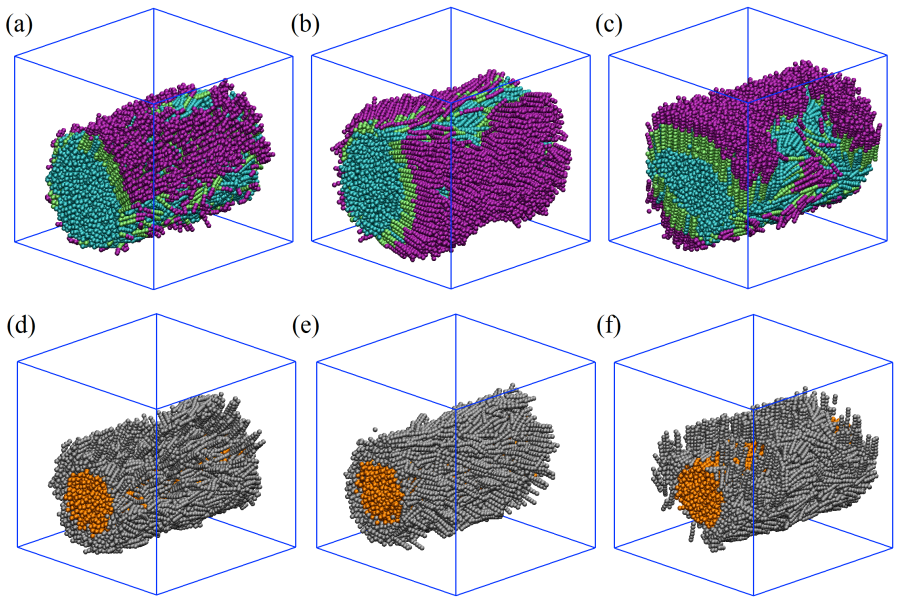

Figure S3. Configurations of LC and 1000 surfactant molecules with S_{head}/S_{tail} = (a) 3/5 (b)7/5 and (c) 5/7 at 0.7 k_BT. Water beads are not shown for clarity. The change in orientation in LCs is due to interactions with surfactants with S_{head}/S_{tail} = (d) 3/5, (e) 7/5, and (f) 5/7. LCs that are located in the core of cylindrical radius ($r_c \leq 5$) are shown in orange, the rest in grey. Water and surfactant beads are not shown for clarity.

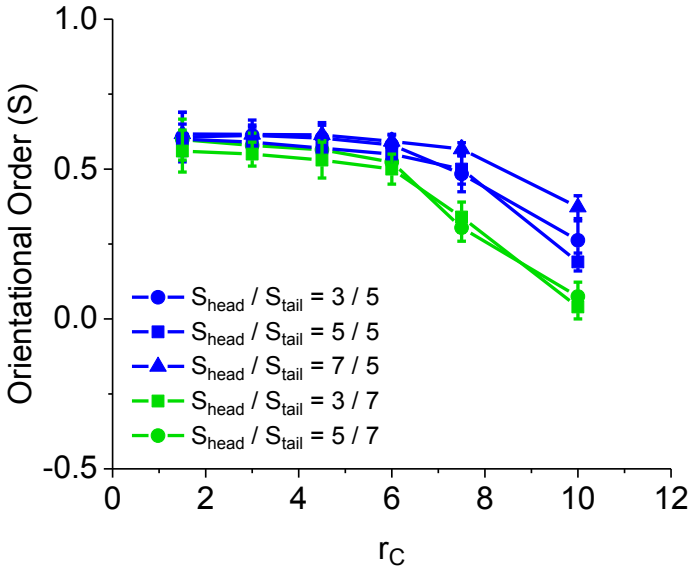

Figure S4. Orientational order as a function of position within the LC cylinder, surface covered by 1000 surfactant molecules. In these simulations $\alpha_{LC\text{-}Stail} = 25$. Blue lines represent surfactants with 5 bead-long tails, green lines represent 7 bead-long tails.