Supplementary Information

Section S1. Simulation Details

In the present study, water (four molecule cluster, W), PB (one monomer) and PEO (one monomer) are represented by bead types P4, C4, SNda, respectively [75,82]. The solvent consists of 90.9% of P4 water beads along with 9.1% of "antifreeze" beads (WF) which are of type BP4 and slightly bigger than the P4 beads. The WF beads are employed to disturb the lattice packing of the uniformly sized solvent beads and decrease the solvent freezing point [76]. The chemical affinities of bead types are described in the paper of Marrink and *et. al.* [75].

The simulations are performed by using the *Gromacs* 2020.2 MD software. First, simulations are conducted to minimize the energy of the initial system by the steepest descent algorithm. This is followed by a short (2 ns in this work) NVT simulation to equilibrate the system at a desired temperature to ensure algorithmic stability. Subsequently, a sufficiently long NPT simulation (production run) is carried out (400 ns in this work). The reason for conducting NVT simulation first is because that velocity generation at the outset of a simulation, which is done by sampling from a Gaussian distribution that yields the mean temperature, is imperfect. When coupled with a barostat, initial velocity distributions thus generated can frequently lead to numerical instabilities. Hence, equilibration is better performed for an NVT ensemble for a short period of time to get the correct the velocity distribution. Proceeding NPT simulations lead to the establishment of the appropriate system density.

The initial simulation box is cubic with a linear dimension of 40 nm. In comparison, the contour length of the longest copolymer chain is 4.07 nm. During the NPT simulation the box size changes to between 39 and 41 nm to match the correct system density.

The reference pressure and temperature are 1 bar and 300K, respectively. A v-rescale thermostat [83] with a time constant of 1.0 ps is used for temperature coupling. Berendsen barostat [84] with a time constant of 4.0 ps is used for isotropic pressure coupling during the NPT simulations. The simulations employ periodic boundary conditions along all three spatial coordinates. The time step for equilibration runs is 20 fs and the run time is 2 ns. The time step for production runs is 40 fs and the run time is up to 400 ns.

Table S1. Parameter values for non-bonded interactions.

Interaction type	ε_{ij}(kJ/mol)	σ_{ij}(nm)
PB-W	2.7	0.47
PB-PB	3.5	0.47
PB-PEO	3.1	0.47
PEO-PEO	3.375	0.43
PEO-W	4	0.47
W-W	5	0.47
W-WF	5.6	0.57
WF-WF	5	0.47
PEO-WF	4	0.47
PB-WF	2.7	0.47

Table S2. Parameter values for bond stretching interactions.

Bond type	b_0(nm)	K_b(kJ/(mol $\cdot$ nm^2))
PB-PB	0.47	1250
PB-PEO	0.47	1250
PEO-PEO	0.33	17000

Table S3. Parameter values for bond bending interactions.

Angle type	θ_0 (degree)	K_θ(kJ/mol)
PB-PB-PB	180	25
PB-PB-PEO	180	25
PB-PEO-PEO	120	50
PEO-PEO-PEO	120	50

**Table S4.** The lognormal fitting parameters for pdf figures in Table 1.

Structure	PEO - μ	PEO - σ	PB - μ	PB- σ
Wormlike micelle	-0.91 $\pm$ 0.08	0.68 $\pm$ 0.06	-0.58 $\pm$ 0.02	0.35 $\pm$ 0.01
Rectangular lamella	-0.87 $\pm$ 0.06	0.54 $\pm$ 0.06	-0.67 $\pm$ 0.02	0.38 $\pm$ 0.01
Disk lamella	-0.88 $\pm$ 0.08	0.64 $\pm$ 0.07	-0.66 $\pm$ 0.02	0.35 $\pm$ 0.02
Cavity micelle	-1.01 $\pm$ 0.05	0.52 $\pm$ 0.05	-0.64 $\pm$ 0.02	0.35 $\pm$ 0.02
Vesicle	-0.92 $\pm$ 0.05	0.48 $\pm$ 0.05	-0.71 $\pm$ 0.02	0.36 $\pm$ 0.02

**Table S5.** The lognormal fitting parameters for figure 5.

| Structure	μ	σ
(a). PB segment	-0.56 $\pm$ 0.01	0.45 $\pm$ 0.01
(b). PEO segment	-0.76 $\pm$ 0.05	0.68 $\pm$ 0.04
(c). PB-PEO chain	0.56 $\pm$ 0.02	0.50 $\pm$ 0.02
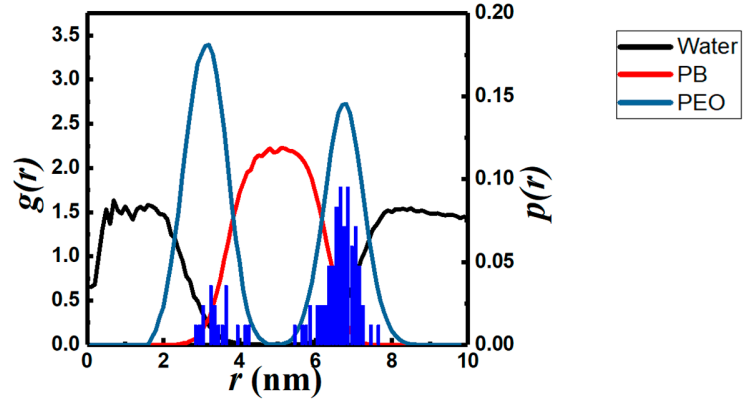
Figure S1. The location of ringlike PEO segments in a vesicle. The histogram shows the probability density function of the location of ringlike PEO segments ($p(r)$). The continuous lines show $g(r)$ for water, PB and PEO. Figure shows that ringlike PEO segments are mainly found in regions in which PB and PEO chains overlap.
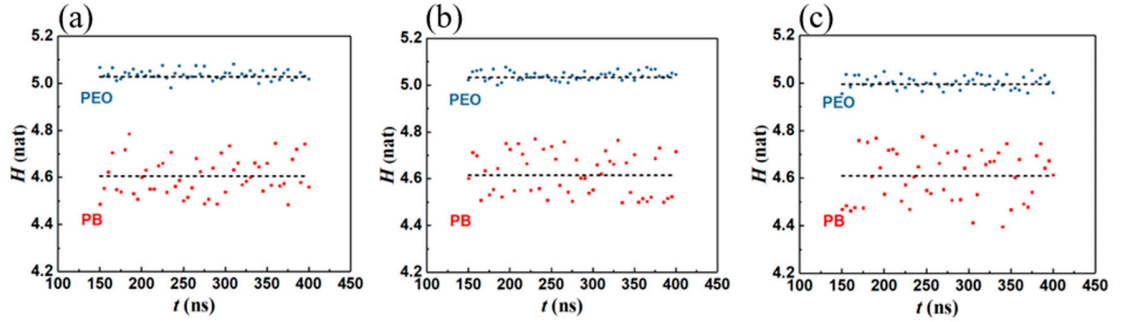

Figure S2. Information entropy vs. time obtained from simulations that start with three different initial copolymer distributions.
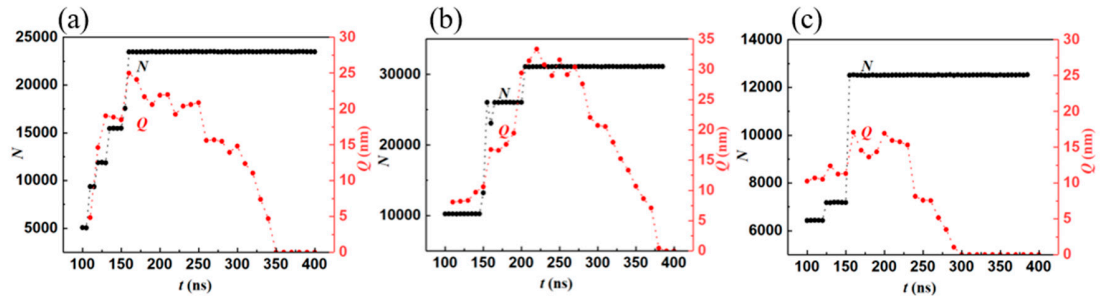
Figure S3. Number of monomers (N) and end-to-end distance (Q) vs. time obtained from simulations that start with three different initial copolymer distributions.
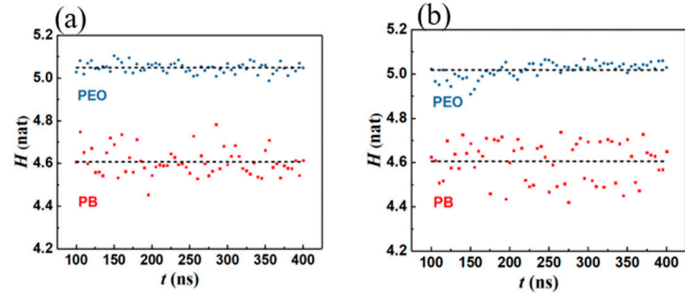
Figure S4. Information entropy vs. time obtained from simulations performed with (a) a 10% reduction and (b) a 10% increase in K_b and K_θ as compared to their values used in the simulations reported in Figure 6.
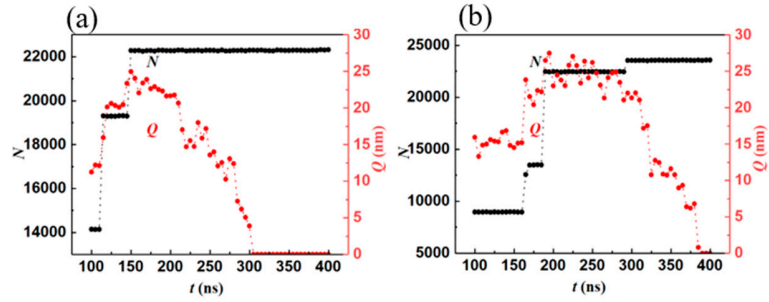
Figure S5. Number of monomers (N) and end-to-end distance (Q) vs. time obtained from simulations performed with (a) a 10% reduction and (b) a 10% increase in K_b and K_θ as compared to their values used in the simulations reported in Figure 3.