Supporting Information

Complexes Comprised of a Dendrimer and a Vesicle: Role of Vesicle Size and the Surface Tension of the Vesicle Membrane

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[Content]

1. The tensionless lipid bilayer vesicles at the equilibrium state.
2. Typical surface tension curve of the amphiphilic molecule membrane against its area peramphiphilic molecule.
3. The dynamical process of the complex between the G5 dendrimer and the small vesicle.
4. The dynamical process of the complex between the G5 dendrimer and the big vesicle.
5. The repulsion parameters in the conservative force.
6. Video

Supporting Information 1

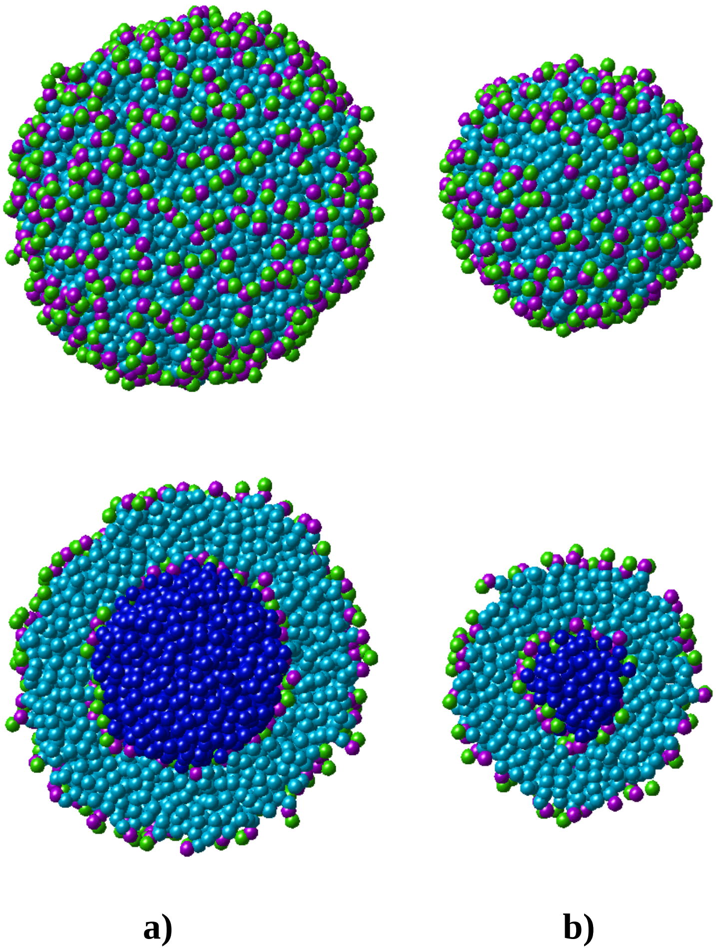


Figure S1. The tensionless lipid bilayer vesicles at the equilibrium state. a) The big vesicle is obtained at the concentration of the amphiphile 9 vol%. b) The small vesicle is obtained at the concentration of the amphiphile 3.6 vol%. The snapshots at bottom show the cross-sectional images of the vesicles. The color code of each bead is the same as that in Figure 1.

Supporting Information 2

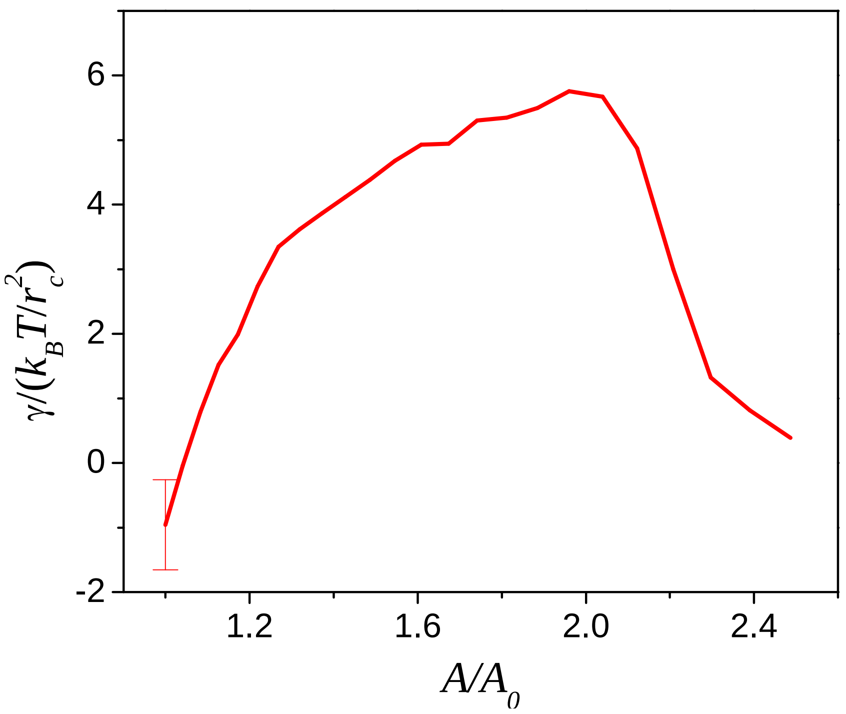
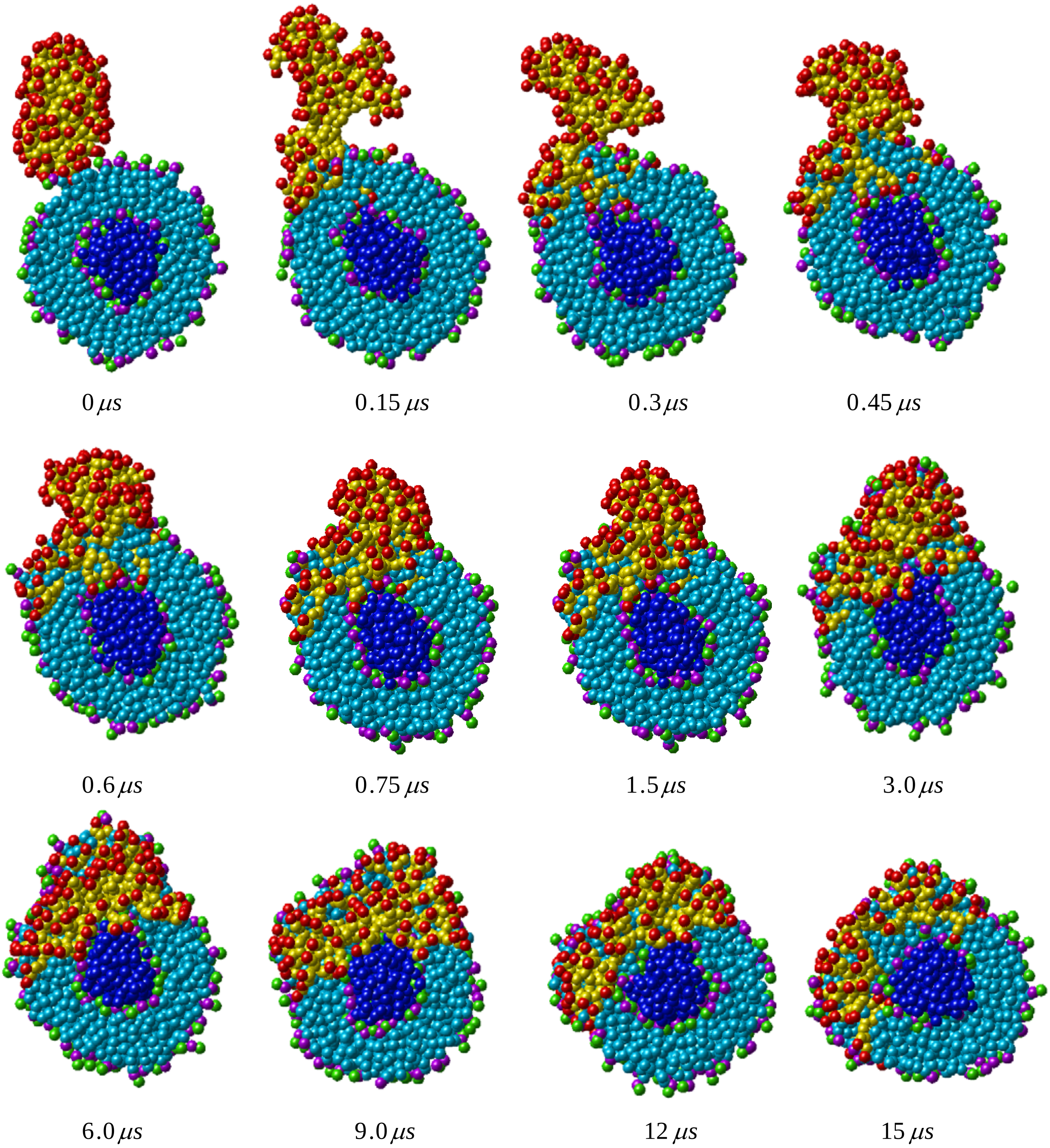


Figure S2. Typical surface tension curve of the membrane of amphiphilic molecules against its area per amphiphilic molecule. The value of the area per amphiphilic molecule at the initial time, i.e., A_0, is $A_0=1.28\,r_c^2$ .All error bars are similar to the one shown.

Supporting Information 3



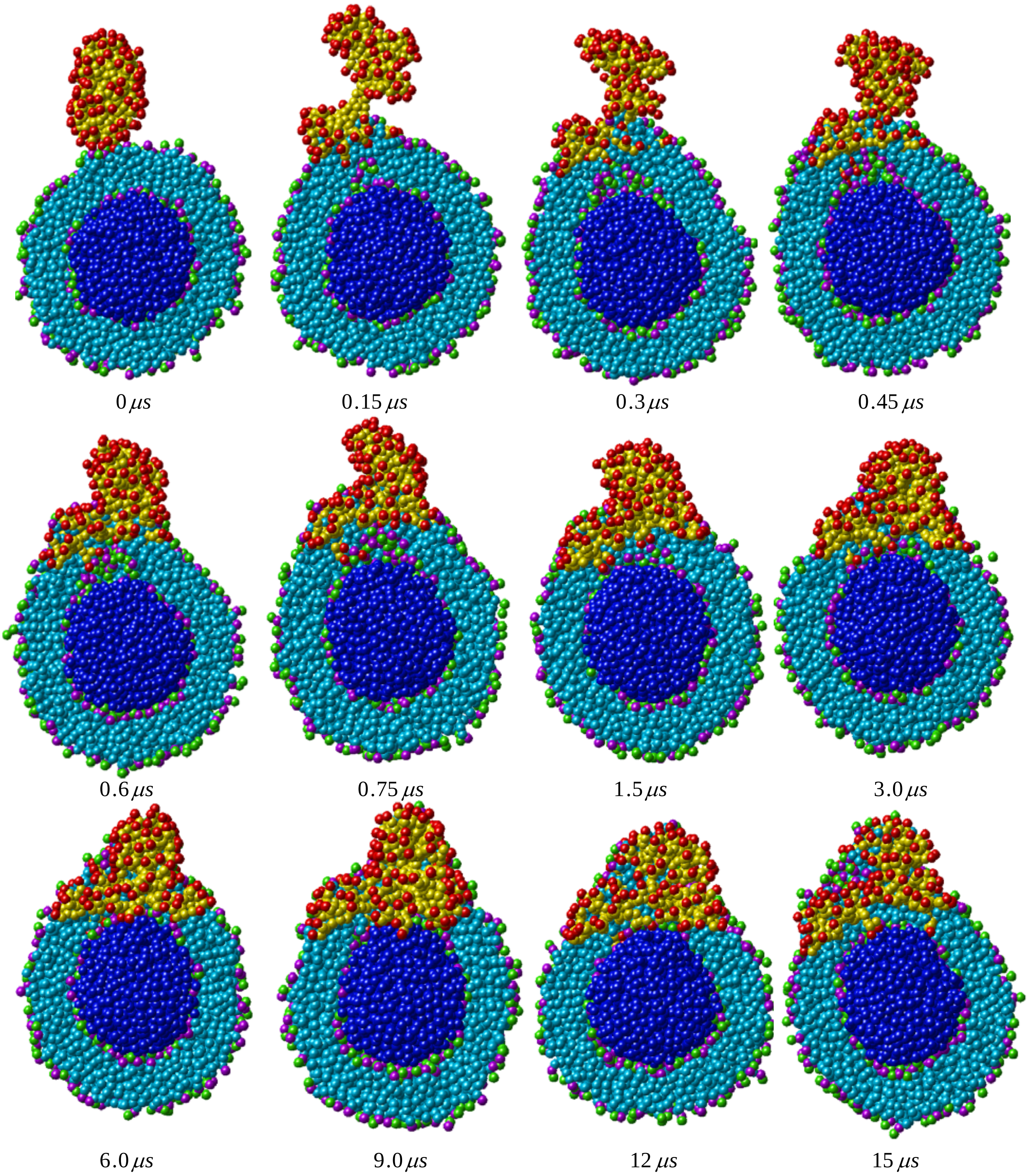
0 μs 0.15 μs 0.3 μs 0.45 μs

0.6 μs 0.75 μs 1.5 μs 3.0 μs

6.0 μs 9.0 μs 12 μs 15 μs

Figure S3. The dynamical process of the complex between the G5 dendrimer and the small vesicle. The color code of each bead is the same as that in Figure 1.

Supporting Information 4



0 μs 0.15 μs 0.3 μs 0.45 μs

0.6 μs 0.75 μs 1.5 μs 3.0 μs

6.0 μs 9.0 μs 12 μs 15 μs

Figure S4. The dynamical process of the complex between the G5 dendrimer and the big vesicle. The color code of each bead is the same as that in Figure 1.

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Table S1. The interaction parameter α_{ij} between different types of beads. The number in each bracket is the corresponding charge of the bead. α_{TU} is the interaction parameters between the hydrophobic dendrimer component and lipid tails, which will be changed in the simulations.

	Lipid head (+1)	Lipid head (-1)	Lipid head (0)	Lipid tail (0)	Solvent bead (0)	Dendrimer bead (+1)	Counterions (-1)	Dendrimer bead (0)
Lipid head (+1)	25	17	22	40	22	15	20	28
Lipid head (-1)	17	25	22	40	22	15	20	28
Lipid head (0)	22	22	25	40	25	15	22	28
Lipid tail (0)	40	40	40	25	80	28	80	α_{TU}
Solvent bead (0)	22	22	25	80	25	20	20	80
Dendrimer bead (+1)	15	15	15	28	20	25	20	28
Counterions (-1)	20	20	22	80	20	20	25	28
Dendrimer bead (0)	28	28	28	α_{TU}	80	28	28	25

Supporting Information 6

Video S1. Process of the complex between the G5 dendrimer and the big vesicle at α_{TU} =15 and . The lipid number and color code are the same as those in Figure1. The number of added solvent beads inside the vesicles N_A/N_0=1.181. Solvent beads outside the vesicle and counterions are not shown for clarity.