Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Manipulating the Interactions between Lipid Bilayer and Triblock Janus Nanoparticle: Insight from Dissipative Particle Dynamics

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SI-1: Interaction parameters

Based on the previous simulation studies[1, 2], we set the interaction parameter α_{ij}, and the detailed values are shown in Table S1. The interaction parameter between the same beads was 25 k_BT. To reflect the hydrophilicity of TJPs, the interaction parameter between the hydrophilic/hydrophobic beads of TJPs and the solvent was set to 20/100 k_BT. The complete interaction parameters (α_{ij}) are reported in Table S1. Previous studies have demonstrated that these parameters are reasonable and convincing. W: water bead, H: hydrophilic bead of lipid, T: hydrophobic bead of lipid, I: hydrophilic bead of TJP, and O: hydrophobic bead of TJP.

Table. S1. Bead-bead interaction parameters α_{ij}.

α_{ij}	H	T	W	I	O
H	25	100	25	25	100
T	100	25	100	100	25
W	25	100	25	20	100
I	25	100	20	25	100
O	100	25	100	100	25

SI-2: Details of simulation system

The triangular packing of beads was adopted to model the smooth surface of nanoparticle, as well as to prevent solvent beads penetrating into nanoparticle, as shown in Fig. S1a. Here, the solid particle model with radius of $2r_c$ is formed by 552 DPD beads. In order to obtain the rational structure of bilayer under zero tension[3, 4], the lipid bilayer system is first simulated. The density profiles of hydrophobic interior and hydrophilic corona in equilibrium demonstrate that the bilayer under zero tension in equilibrium is flat and complete, and the interior and exterior force of the lipid bilayer are balanced, as shown in Fig. S1b. After the bilayer system reach equilibrium, each TJP was placed at $10r_c$ above the balanced bilayer to conduct following simulation.

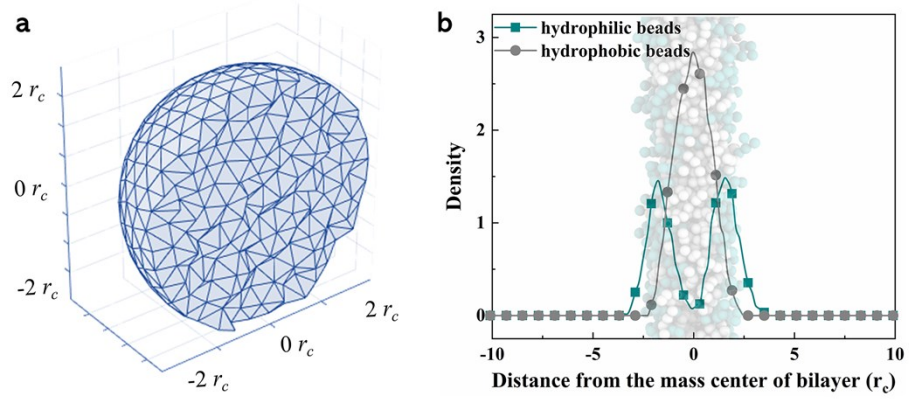

Fig. S1 (a) Solid nanoparticle model based on the triangular packing of beads. (b) Density profile of hydrophilic/hydrophobic beads of lipid bilayer in equilibrium state.

SI-3: Detachment process of triblock Janus nanoparticle

Fig. S2 depicts the detachment process of TJP. The detachment of TJP is accompanied by the bending deformation of membrane. After the penetration of TJP, the bilayer starts to reseal itself.

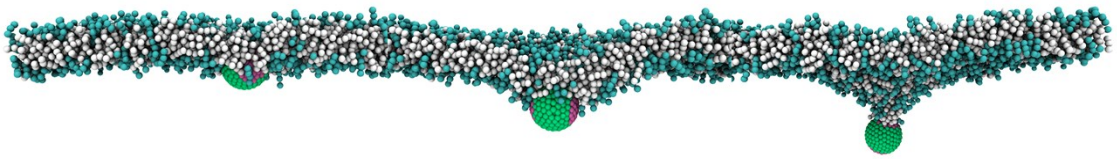

Fig. S2 Detachment of TJP from bilayer, taking $B_1A_3B_1$ TJP as example.

References

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