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Nanoparticle encapsulation in vesicles formed by amphiphilic diblock copolymers

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Table S1 Summary of the vesicle sizes, cavity sizes and corresponding wall thicknesses with various B-block length n_B for A_2B_n diblock copolymers with $a_{BS} = 130$. The concentration of nanoparticle ϕ_P is fixed at 0.01.

sample	R_{in}	d	R_{out}
A_2B_{10}	2.802610	5.534639	8.337249
A_2B_{11}	2.471230	5.844953	8.316184
A_2B_{12}	2.233170	6.073174	8.306344
A_2B_{13}	1.981948	6.320687	8.302635
A_2B_{14}	1.662791	6.628279	8.291070
A_2B_{15}	1.365275	6.917073	8.282348

Table S2 Summary of the averaged distance of each two nanoparticles r_{PP} with various B-block length n_B for A_2B_n diblock copolymers with $a_{BS}=130$. The concentration of nanoparticle ϕ_P is fixed at 0.01.

sample	r_{PP}
A_2B_{10}	8.5500
A_2B_{11}	8.1860
A_2B_{12}	7.6410
A_2B_{13}	7.3680
A_2B_{14}	6.6400
A_2B_{15}	6.0950

Table S3 Summary of the vesicle sizes, cavity sizes and corresponding wall thicknesses with different concentrations of nanoparticle ϕ_P for A_2B_{10} di-block copolymers with $a_{BS}=130$.

ϕ_P	R_{in}	d	R_{out}
0	3.257944	4.939502	8.197446
0.01	2.802610	5.537695	8.340305
0.02	2.454276	6.037666	8.491942
0.03	2.336723	6.390369	8.727092
0.04	2.056502	6.861687	8.918189
0.05	1.591532	7.523134	9.114667
0.06	1.048284	8.340261	9.388544
0.07	0.992603	8.652660	9.645263

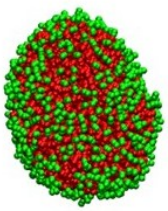
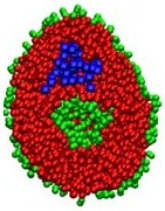
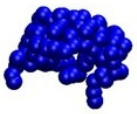
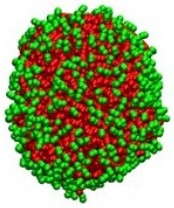
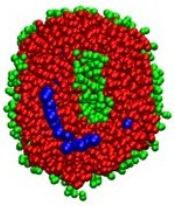
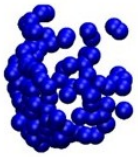
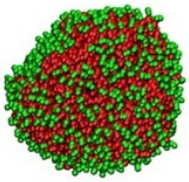
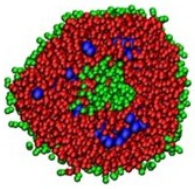
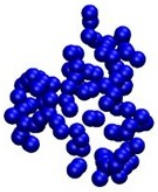
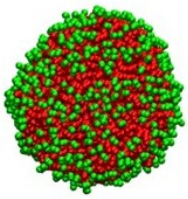
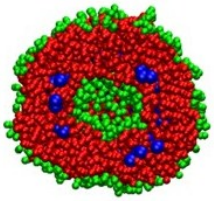
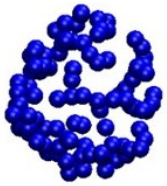
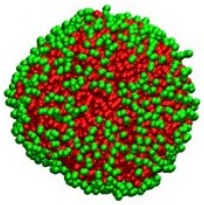
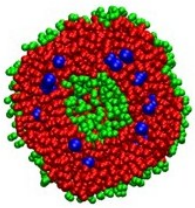
	Aggregate	Slice	Nanoparticle
$a_{PP} = 35$			
$a_{PP} = 40$			
$a_{PP} = 45$			
$a_{PP} = 50$			
$a_{PP} = 55$			

Fig. S1 Effects of the interaction parameter a_{PP} on the distribution of nanoparticle in vesicles formed by A_2B_{10} diblock copolymers with $a_{BS} = 130$ The concentration of nanoparticle ϕ_P is fixed at 0.01.

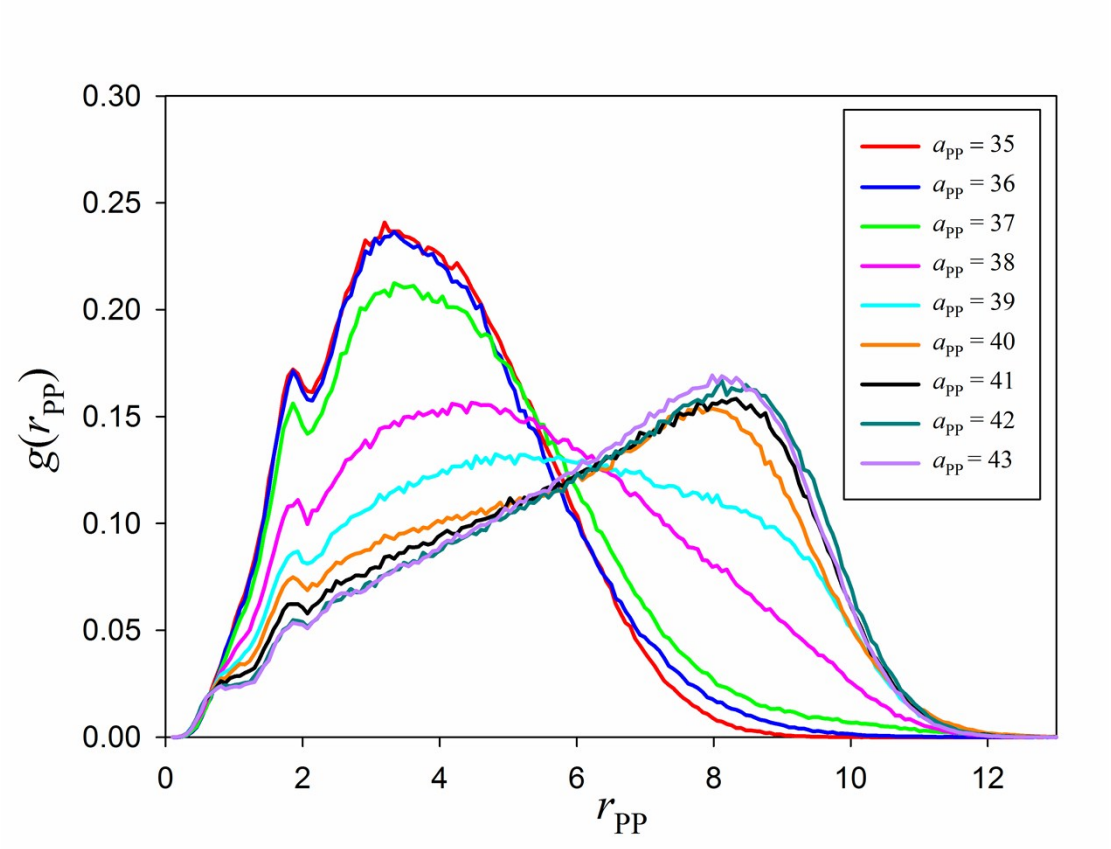


Fig. S2 Radial distribution function $g(r_{PP})$ of nanoparticles within the aggregates, self-assembled from A_2B_{10} diblock copolymers with $a_{BS} = 130$, in terms of interaction parameters a_{PP}. The concentration of nanoparticle ϕ_P is fixed at 0.01.

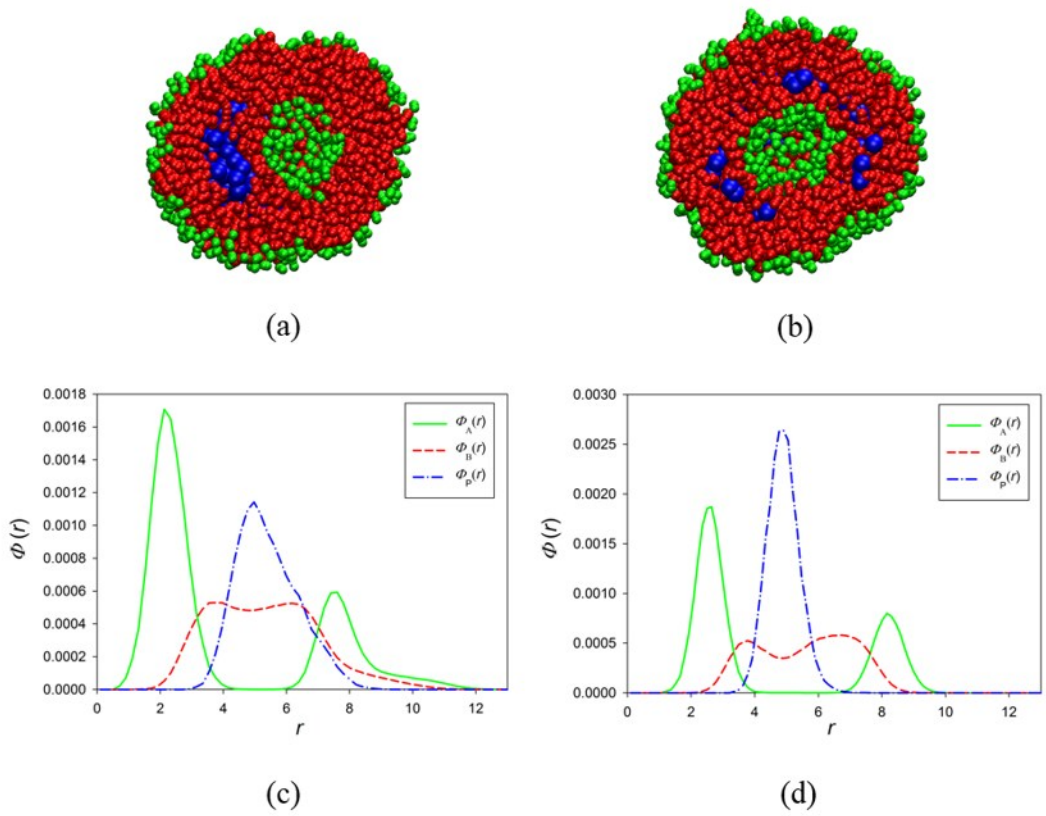


Fig. S3 Cross-sections of aggregates formed by A_2B_{10} diblock copolymers with $a_{BS}=130$ and $a_{PP}=35$ (a), $a_{PP}=50$ (b). The green, red, and blue beads represent A, B and P beads, respectively. (c), (d) Radial density distributions of the hydrophilic block $\Phi_A(r)$ (green solid line), the hydrophobic block $\Phi_B(r)$ (red dashed line) and the nanoparticles $\Phi_P(r)$ (blue dash-dotted line) as a function of the distance r from the geometric center of the aggregates corresponding to (a), (b). Note that normalizations have been chosen such that $4\pi\int_0^R \Phi_A(r)r^2dr=1$, $4\pi\int_0^R \Phi_B(r)r^2dr=1$ and $4\pi\int_0^R \Phi_P(r)r^2dr=1$. The concentration of nanoparticle ϕ_P is fixed at 0.01.

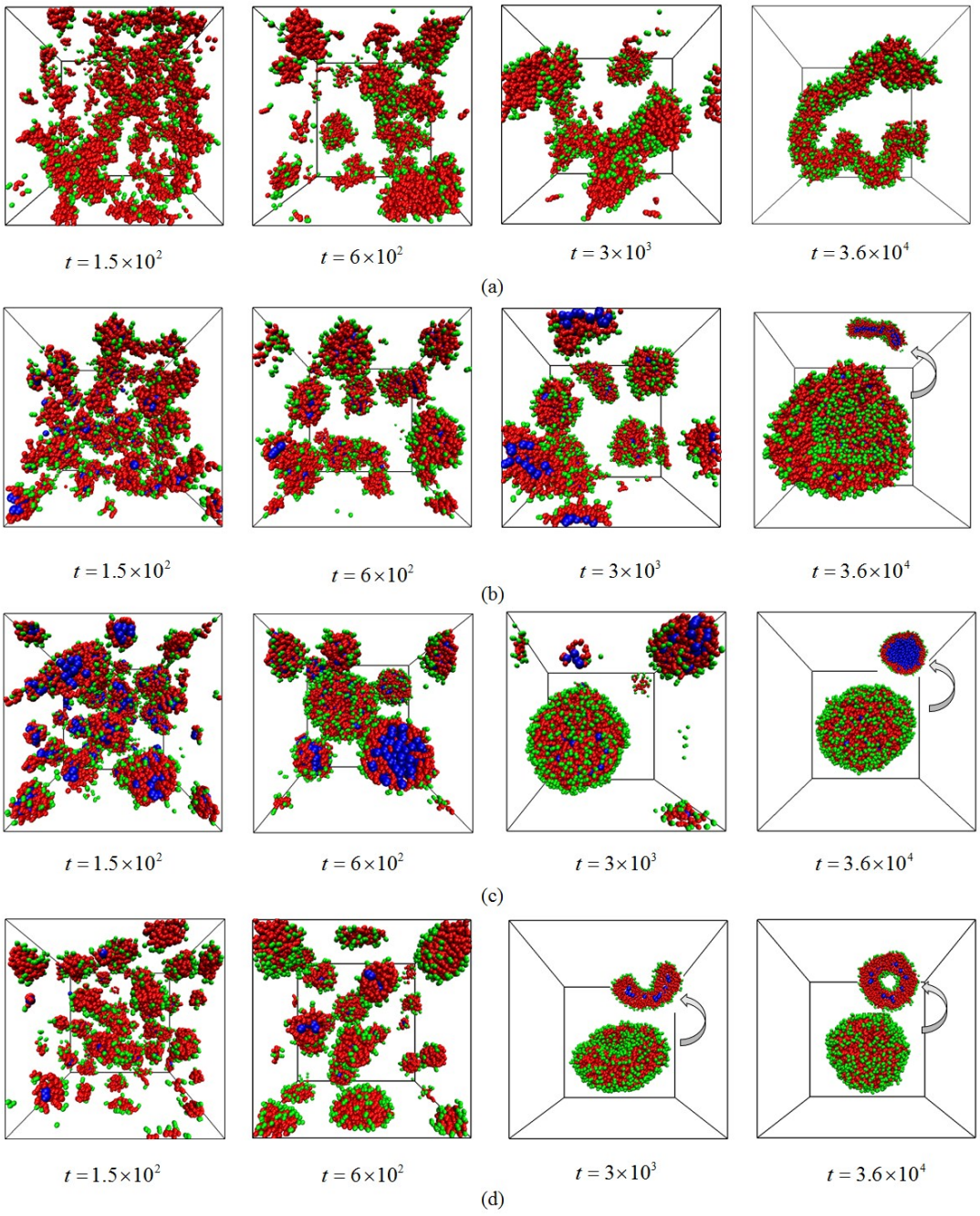


Fig. S4 Snapshots of formation pathways of the representative aggregates (a) rod-like micelle; (b) disk-like micelle; (c) spherical micelle and (d) vesicle. The arrow points to the cross-sectional slice of the aggregate.

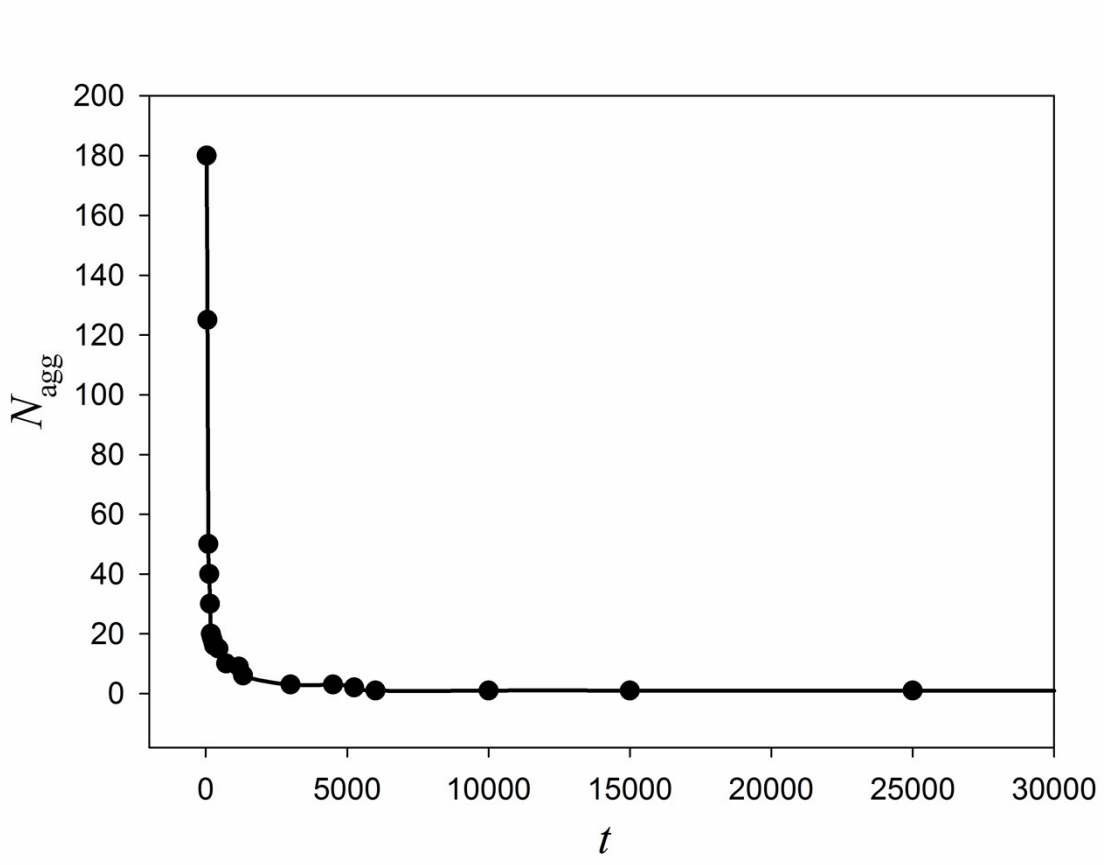


Fig. S5 Number of the aggregate formed by A_2B_{10} diblock copolymers with $a_{BS} = 130$ and $\phi_P = 0.01$ in a cubic box (30^3) as a function of simulation time.

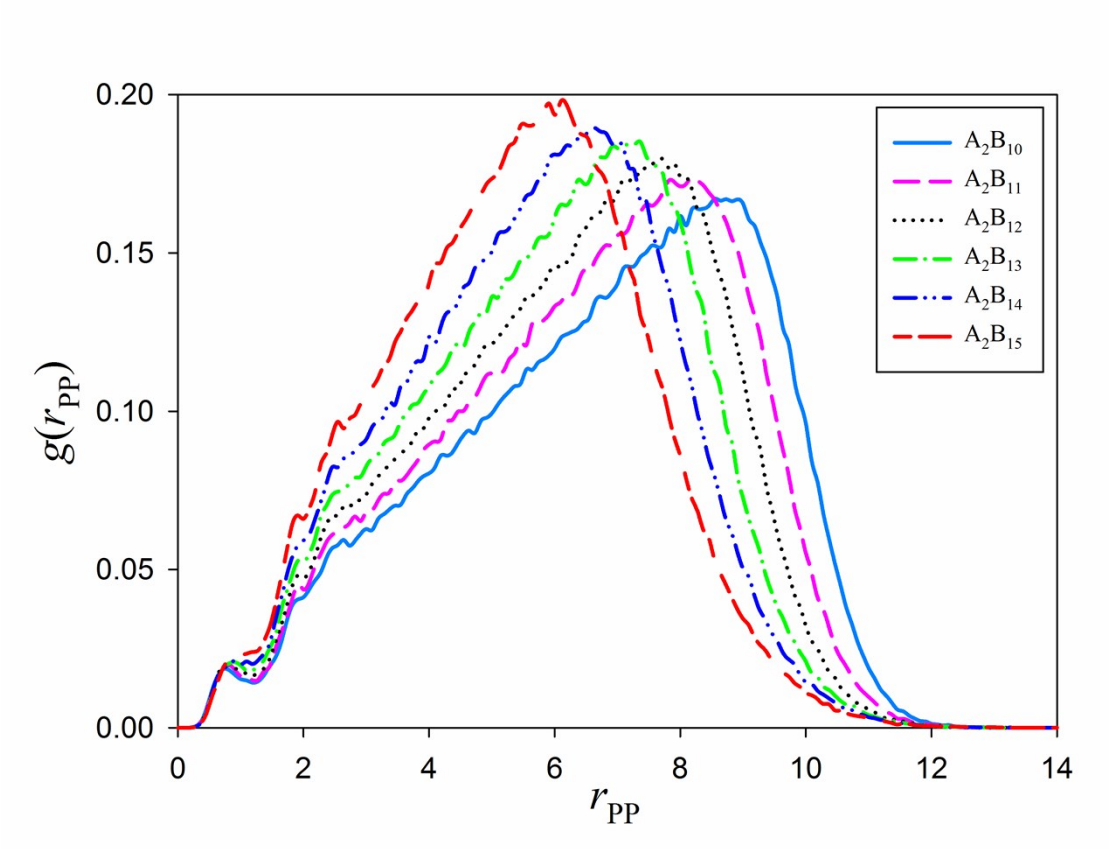


Fig. S6 Radial distribution function $g(r_{PP})$ of nanoparticles within the membrane of vesicles, self-assembled from A_2B_n diblock copolymers with $a_{BS} = 130$. The concentration of nanoparticle ϕ_P is fixed at 0.01.