Electronic Supplementary Information

Controlling the Localization of Nanoparticles in Assemblies of Amphiphilic Diblock Copolymers

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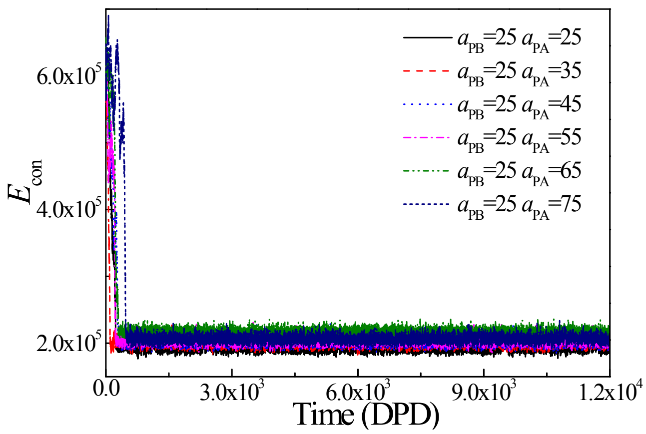
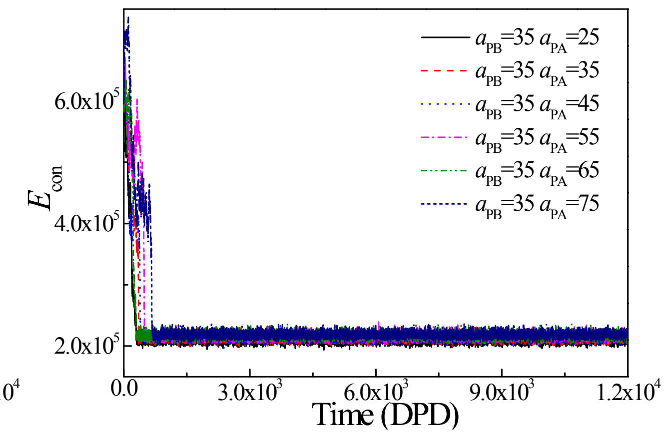
Supporting Information

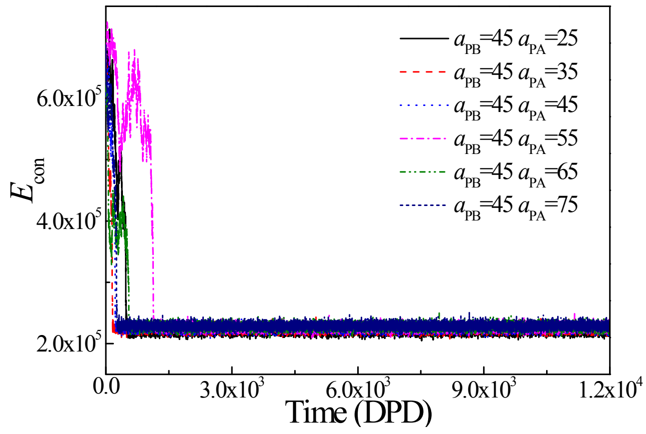
Figure S1 Conservative energy of the diblock copolymer tethered nanoparticles versus simulation time with different a_{PA} and a_{PB}.



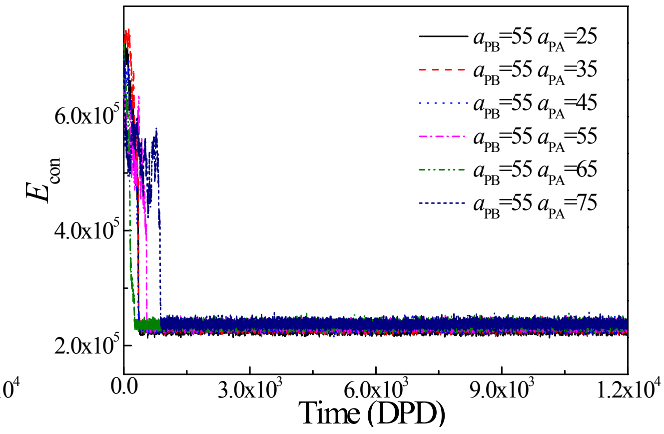
(a)



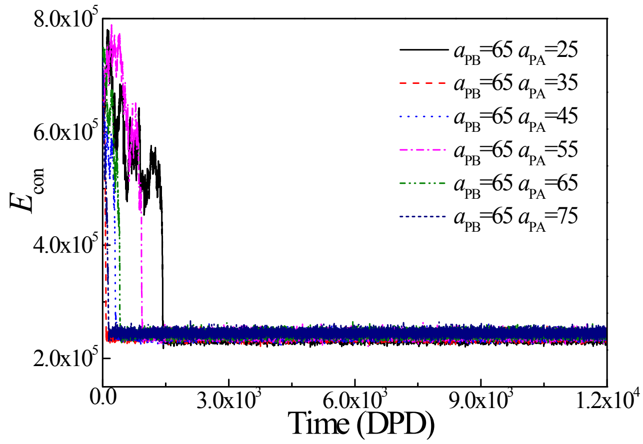
(b)



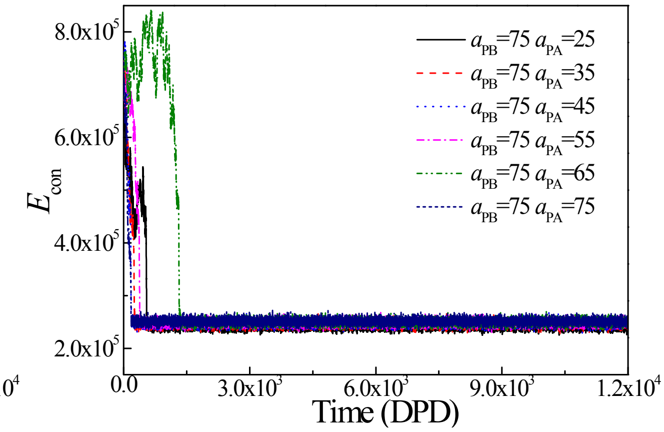
(c)



(d)



(e)



(f)

Table S1 The aggregation number of the aggregates in different size box with different a_{PA} and a_{PB} as the system reaches equilibrium.

a_{ij}	$L^3=25^3$	$L^3=30^3$
a_{PB} =25 a_{PA}=25	191, 43	182,160,63
a_{PB} =25 a_{PA}=35	90, 81, 63	175,103,83,44
a_{PB} =25 a_{PA}=45	212, 22	123,119,72,68, 23
a_{PB} =25 a_{PA}=55	124, 110	180,139,55,20,11
a_{PB} =25 a_{PA}=65	120, 114	165,142,70,28
a_{PB} =25 a_{PA}=75	91,52,44,33,14	145,111,72,54,23

a_{ij}	$L^3=25^3$	$L^3=30^3$

a_{PB} =35 a_{PA}=25	85,75,74	133,106,79,75,12
a_{PB} =35 a_{PA}=35	202,32	91,79,68,68,51,35,13
a_{PB} =35 a_{PA}=45	76,68,62,28	198,81,50,33,27,16
a_{PB} =35 a_{PA}=55	214,20	169,80,56,40,28,25,7
a_{PB} =35 a_{PA}=65	164,70	283,90,32
a_{PB} =35 a_{PA}=75	234	180,111,43,37,34

a_{ij}	$L^3=25^3$	$L^3=30^3$
a_{PB} =45 a_{PA}=25	173,44,17	243,119,43
a_{PB} =45 a_{PA}=35	116,74,44	231,63,63,48
a_{PB} =45 a_{PA}=45	143,91	172,84,60,36,28,25
a_{PB} =45 a_{PA}=55	131,55,48	216,76,55,38,20
a_{PB} =45 a_{PA}=65	181,53	174,72,66,58,35
a_{PB} =45 a_{PA}=75	234	264,60,59,22

a_{ij}	$L^3=25^3$	$L^3=30^3$
a_{PB} =55 a_{PA}=25	117,62,35,20	161,117,79,28,11
a_{PB} =55 a_{PA}=35	186,29,19	312,93
a_{PB} =55 a_{PA}=45	175,59	139,90,76,68,32
a_{PB} =55 a_{PA}=55	118,116	225,177,3
a_{PB} =55 a_{PA}=65	127,85,22	187,184,18,16
a_{PB} =55 a_{PA}=75	160,74	175,104,91,35

a_{ij}	$L^3=25^3$	$L^3=30^3$
a_{PB} =65 a_{PA}=25	171,27,25,11	285,91,19,10
a_{PB} =65 a_{PA}=35	192,42	315,54,36
a_{PB} =65 a_{PA}=45	234	247,104,54
a_{PB} =65 a_{PA}=55	234	103,103,89,82,28
a_{PB} =65 a_{PA}=65	190,44	203,160,42

a_{PB} =65 a_{PA}=75	234	49,135,221

a_{ij}	$L^3=25^3$	$L^3=30^3$
a_{PB} =75 a_{PA}=25	127,107	293,93,19
a_{PB} =75 a_{PA}=35	234	222,113,45,25
a_{PB} =75 a_{PA}=45	170,26,23,15	211,117,77
a_{PB} =75 a_{PA}=55	145,89	144,122,70,69
a_{PB} =75 a_{PA}=65	106,66,62	161,86,67,60,31
a_{PB} =75 a_{PA}=75	234	287,65,42,11

Table S2 Calculated the average mean square of the end-to-end distance of tethered copolymer chain and S_c with various a_{PA} as fixed a_{PB} = 25

a_{PA}	R_e^2	S_c
25	1.483	1.111
35	1.532	1.129
45	1.555	1.137
55	1.576	1.145
65	1.590	1.150
75	1.595	1.152

Note: The R_{e0}^2 of the tethered chain is 1.202.

Table S3 Calculated the average mean square of the end-to-end distance of tethered copolymer chain and S_c with various a_{PB} as fixed a_{PA} = 25

a_{PB}	R_e^2	S_c
25	1.483	1.111
35	1.500	1.117
45	1.504	1.119
55	1.523	1.126
65	1.520	1.125

75	1.529	1.128

Note: The R_{e0}^2 of the tethered chain is 1.202.

Table S4 Calculated the average mean square of the end-to-end distance of solvophobic block B and S_c with various a_{PA} and a_{PB}

a_{PA} =a_{PB}	R_e^2	S_c
25	0.692	0.955
35	0.686	0.951
45	0.681	0.947
55	0.652	0.927
65	0.653	0.928
75	0.642	0.920

Note: The R_{e0}^2 of the solvophobic B-block is 0.759.

Table S5 The Mode A number fraction of the obtained spherical micelle at t = 15000 with different a_{PA} and a_{PB}

	N_{agg}	N_A	N_B	Φ_A
a_{PB} =25 a_{PA}=25	191	75	116	0.393
a_{PB} =25 a_{PA}=25	43	17	26	0.395
a_{PB} =25 a_{PA}=35	81	35	46	0.432
a_{PB} =25 a_{PA}=35	90	37	53	0.411
a_{PB} =25 a_{PA}=35	63	27	36	0.428

Note: N_{agg} is the number of copolymer in one aggregate. N_A and N_B are the number of copolymer with Mode A and Mode B in the aggregate, respectively. Φ_A is the number fraction of Mode A of the obtained aggregate.

Table S6 The Mode A number fraction of the obtained vesicle at t = 15000 with different a_{PA} and a_{PB}

	N_{agg}	N_A	N_B	Φ_A
a_{PB} =25 a_{PA}=55	124	50	74	0.403
a_{PB} =25 a_{PA}=55	110	46	64	0.418
a_{PB} =25 a_{PA}=65	114	53	61	0.465

a_{PB} =25 a_{PA}=65	120	58	62	0.483

Note: N_{agg} is the number of copolymer in one aggregate. N_A and N_B are the number of copolymer with Mode A and Mode B in the aggregate, respectively.

Table S7 The Mode A number fraction of the obtained disk-like micelles at t = 15000 with different a_{PA} and a_{PB}

	N_{agg}	N_A	N_B	Φ_A
a_{PB} =35 a_{PA}=45	76	0	76	0
a_{PB} =35 a_{PA}=45	68	0	68	0
a_{PB} =35 a_{PA}=45	62	0	62	0
a_{PB} =35 a_{PA}=55	214	0	214	0
a_{PB} =45 a_{PA}=45	143	0	143	0
a_{PB} =45 a_{PA}=45	91	0	91	0

Note: N_{agg} is the number of copolymer in one aggregate. N_A and N_B are the number of copolymer with Mode A and Mode B in the aggregate, respectively. Φ_A is the number fraction of Mode A of the obtained aggregate.

Table S8 The Mode A number fraction of the obtained rod-like micelle at t = 15000 with different a_{PA} and a_{PB}

	N_{agg}	N_A	N_B	Φ_A
a_{PB} =75 a_{PA}=25	127	0	127	0
a_{PB} =75 a_{PA}=25	107	0	107	0
a_{PB} =75 a_{PA}=65	62	0	62	0
a_{PB} =75 a_{PA}=65	66	0	66	0
a_{PB} =75 a_{PA}=65	106	0	106	0

Note: N_{agg} is the number of copolymer in one aggregate. N_A and N_B are the number of copolymer with Mode A and Mode B in the aggregate, respectively. Φ_A is the number fraction of Mode A of the obtained aggregate.