Binding to semiflexible polymers: a novel method to control the structures of small numbers of building blocks

Dong Zhang[1], Linxi Zhang[2, *)]

[1]*Department of Physics, Zhejiang University, Hangzhou 310027, China*

[2]*Department of Physics, Wenzhou University, Wenzhou 325035, China*

[*] Corresponding author. E-mail: lxzhang@zju.edu.cn.

Figure Captions

Figure S1 (a) Measurements of some related parameters in a simulation run and the comparisons of the bending and binding energies between the bridging (domain A) and the aggregating (domain B) phases in the two-particle case for semiflexible chains with a moderate bending energy $b = 140k_BT$. (b) Typical simulation snapshots at different simulation times: (i) $t = 1.5\times10^5\tau_0$; (ii) $t = 3\times10^5\tau_0$; (iii) $t = 4.5\times10^5\tau_0$; and (iv) $t = 5.5\times10^5\tau_0$.

Figure S2. The dynamic process of the formation of a linear contact aggregation structure for small numbers of particles at moderate polymer stiffness $b = 140k_BT$. Here $N_p = 8$.

Figure S3. A star semiflexible chain model used to explore the self-woven helical cage of semiflexible chains, in which there are 10 arms and each arm contains *N=200* monomers.

Figure S4 (a) Small numbers of binding particles ($N_p = 20$) are aggregated in a linear contact manner to form a rod-like structure, in which the star chains wrap around the rod-like structure to form a cage. (b) Main view of a self-woven helical cage on the XZ plane, where different arms are represented by different colors.

Figure S5. A possible structure transition for small numbers of regular tetrahedron building blocks when the polymer bending energies are increased.

Figure S1(a)

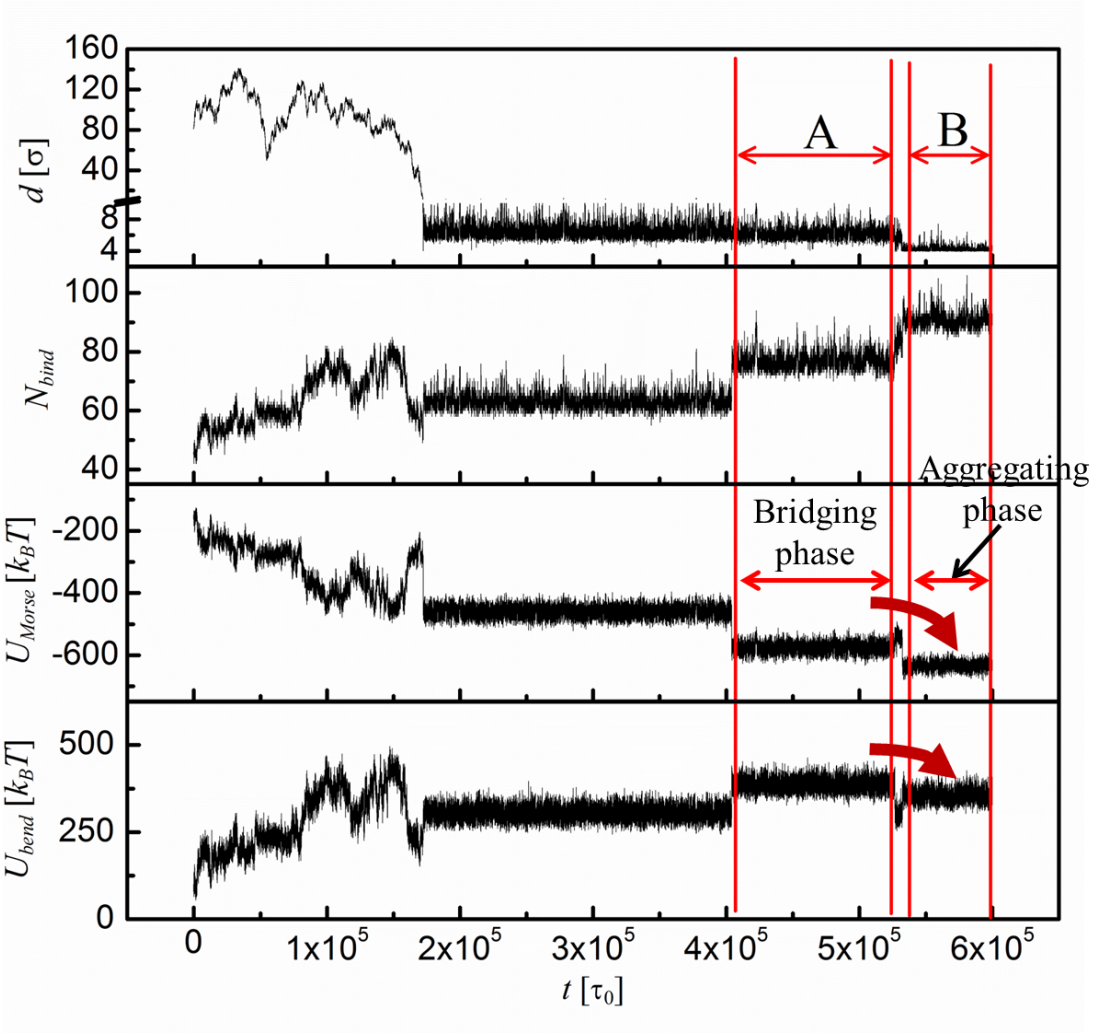
160
120
80
40
8
4
d [σ]
A
B
100
80
60
40
N_bind
Aggregating
phase
Bridging
phase
-200
-400
-600
U_Morse [k_BT]
500
250
0
U_bend [k_BT]
0
1x10^5
2x10^5
3x10^5
4x10^5
5x10^5
6x10^5
t [τ_0]

Figure S1(b)

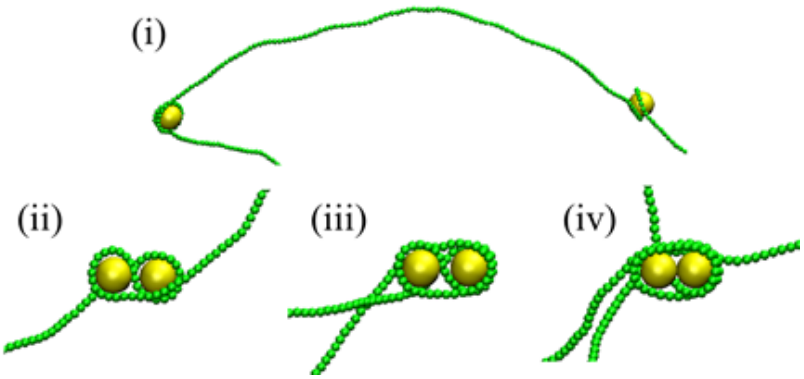

Figure S2

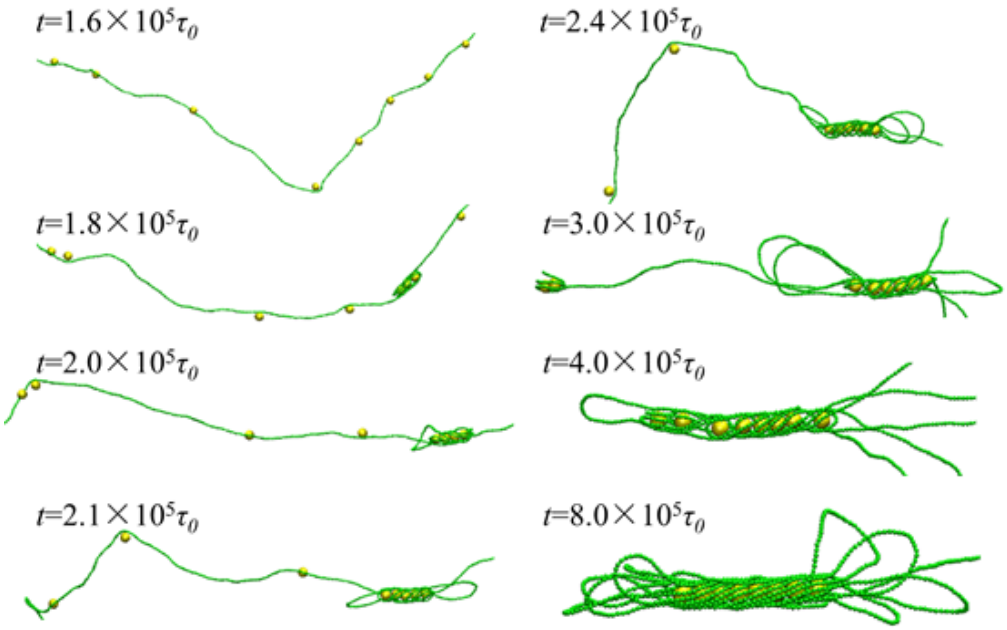
t=1.6×10$^5\tau_0$
t=2.4×10$^5\tau_0$
t=1.8×10$^5\tau_0$
t=3.0×10$^5\tau_0$
t=2.0×10$^5\tau_0$
t=4.0×10$^5\tau_0$
t=2.1×10$^5\tau_0$
t=8.0×10$^5\tau_0$

Figure S3

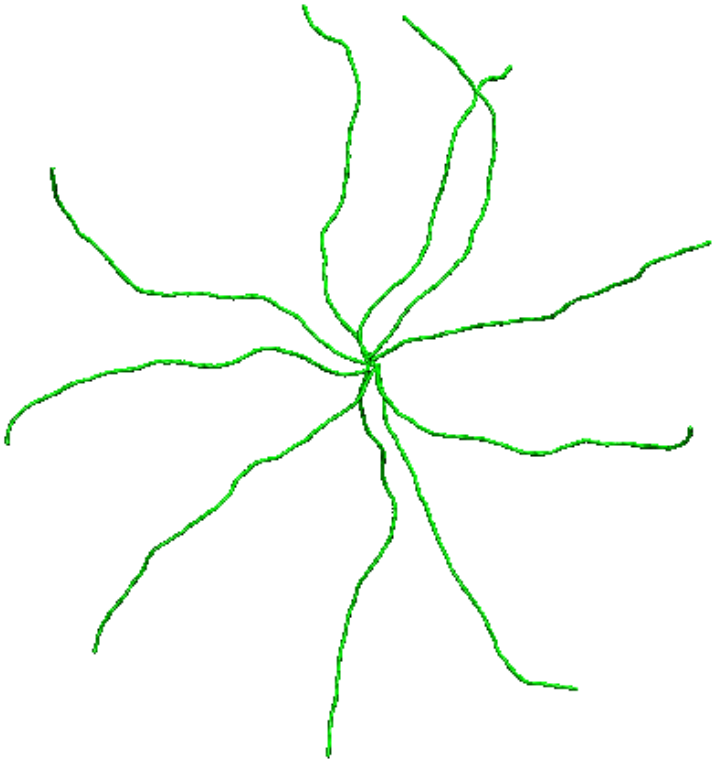

Figure S4(a)

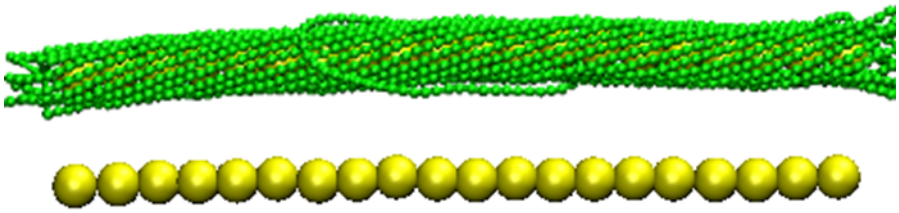

Figure S4(b)

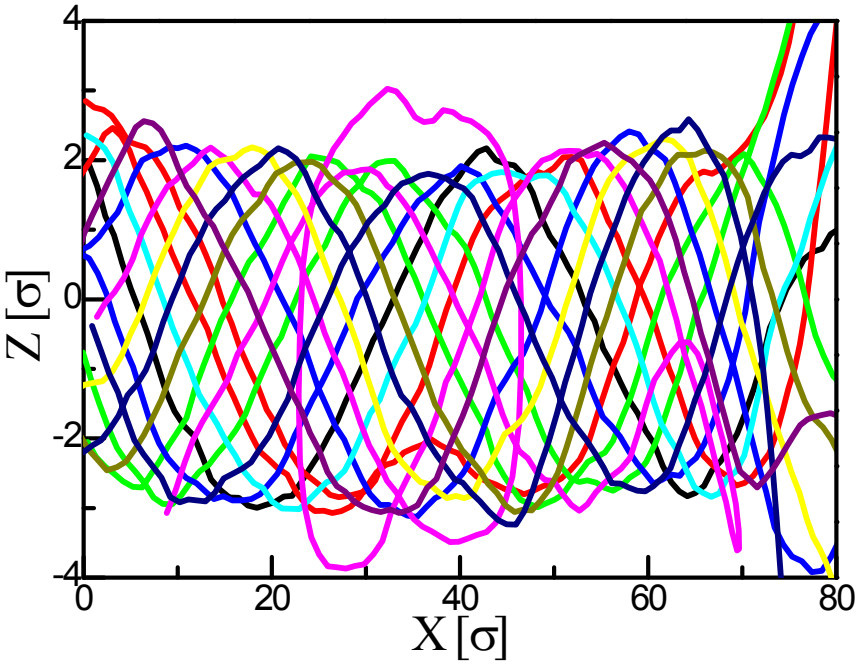

Figure S5

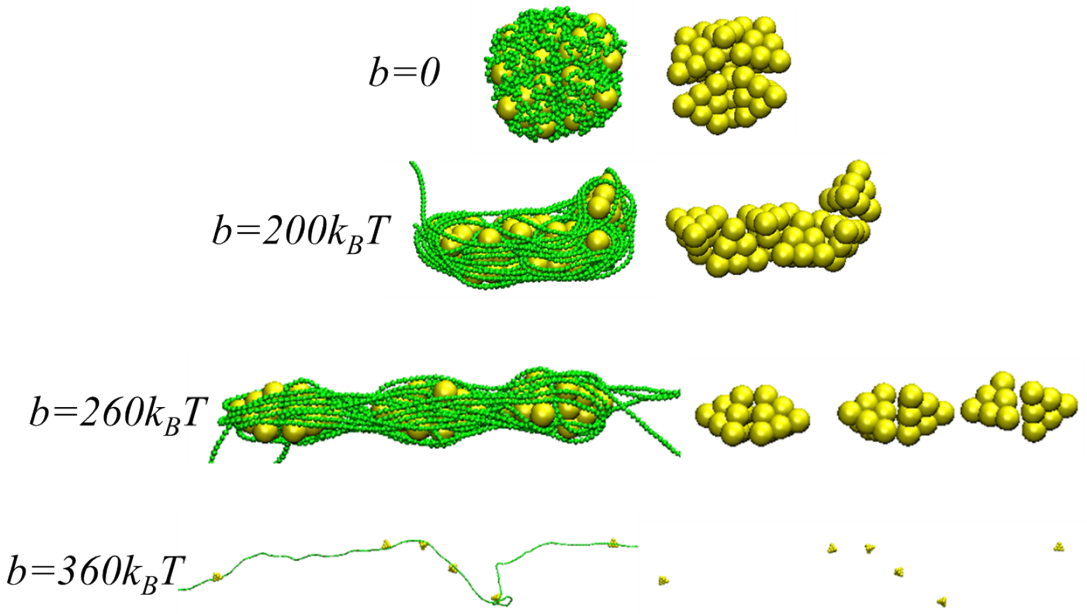

Table S1 Related simulation parameters used to explore the structures of non-spherical building blocks.

	Number of constructed particles per building block (N_c)	Number of building blocks (N_b)	Number of polymer monomers (N)	Binding interaction (D_0/k_BT)
Rod	5	3	1000	10
Regular triangle	6	5	1500	8
Regular hexagon	7	5	1500	8
Regular tetrahedron	10	6	1500	5