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

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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) $t = 1.5 \times 10^5\tau_0$; (ii) $t = 3 \times 10^5\tau_0$; (iii) $t = 4.5 \times 10^5\tau_0$; and (iv) $t = 5.5 \times 10^5\tau_0$.

**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)
Figure S1(b)

(i)  
(ii)  
(iii) 
(iv)
Figure S2

\[ t = 1.6 \times 10^5 \tau_0 \]

\[ t = 1.8 \times 10^5 \tau_0 \]

\[ t = 2.0 \times 10^5 \tau_0 \]

\[ t = 2.1 \times 10^5 \tau_0 \]

\[ t = 2.4 \times 10^5 \tau_0 \]

\[ t = 3.0 \times 10^5 \tau_0 \]

\[ t = 4.0 \times 10^5 \tau_0 \]

\[ t = 8.0 \times 10^5 \tau_0 \]
Figure S3
Figure S4(a)
Figure S4(b)
Figure S5

- $b=0$
- $b=200k_B T$
- $b=260k_B T$
- $b=360k_B T$
Table S1 Related simulation parameters used to explore the structures of non-spherical building blocks.

<table>
<thead>
<tr>
<th></th>
<th>Number of constructed particles per building block ((N_c))</th>
<th>Number of building blocks ((N_b))</th>
<th>Number of polymer monomers ((N))</th>
<th>Binding interaction ((D_r/k_B T))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod</td>
<td>5</td>
<td>3</td>
<td>1000</td>
<td>10</td>
</tr>
<tr>
<td>Regular triangle</td>
<td>6</td>
<td>5</td>
<td>1500</td>
<td>8</td>
</tr>
<tr>
<td>Regular hexagon</td>
<td>7</td>
<td>5</td>
<td>1500</td>
<td>8</td>
</tr>
<tr>
<td>Regular tetrahedron</td>
<td>10</td>
<td>6</td>
<td>1500</td>
<td>5</td>
</tr>
</tbody>
</table>