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Supplementary Information (SI) for Soft Matter.

Sliding dynamics of multi-rings on semiflexible polymer in poly[*n*]catenanes

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S1. The probability density distribution function P(S) of central cyclic polymer

In our simulations, we first calculated the probability density distribution function of radius of gyration $P_0(R_g)$ with different bending energy of central rings in equilibrated state, and made them as the criterion for sampling the fixed rings. We choose 500 equilibrated conformations at random and then also calculate the probability density distribution function of radius of gyration $P(R_g)$.

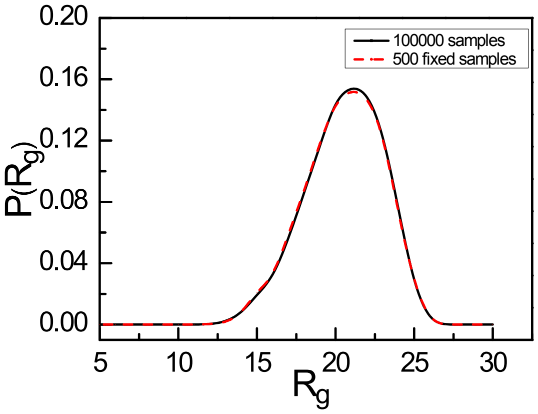

Fig.S1. The probability density distribution function of radius of gyration $P(R_g)$ vs R_g for the central cyclic polymer with k_b=10. Here solid line denotes $P(R_g)$ of the non-fixed central rings with 100000 samples and dotted line represents 500 samples for the fixed central ring. Here N_S=10.

If the relative difference between $P_0(R_g)$ and $P(R_g)$ is less than 5% for different R_g, i.e, $|P_0(R_g)-P(R_g)|/P_0(R_g)<5\%$ for $0<R_g<R_{g,max}$, these 500 initial central ring polymers can be fixed and the diffusion coefficients of sliding dynamics are averaged in those 500 simulation runs. Figure S1 shows that the distribution function $P(R_g)$ of our 500 fixed samples as a function of R_g for the ring with k_b=10.

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S2. Persistence length (l_P) and bond vector correlation function (C_1) of central ring polymer

Persistence length is an important parameter to describe the conformations of semiflexible polymer. We calculated the persistence length of central cyclic polymer according to the exponential decay of orientation correlation in a chain [1-3]

$$< u(r) \cdot u(0) > \; = e^{-r/l_P} \qquad \text{(S1)}$$

Where **u**(r) and **u**(0) are the unit bond vectors which are separated by a contour distance *r* along the chain, and the brackets <> represent an average of overall starting position and chain configurations. The bond vector correlation function C_1 is defined as[4]

$$C_1 = < b_i \cdot b_{i+1} >$$

(S2)

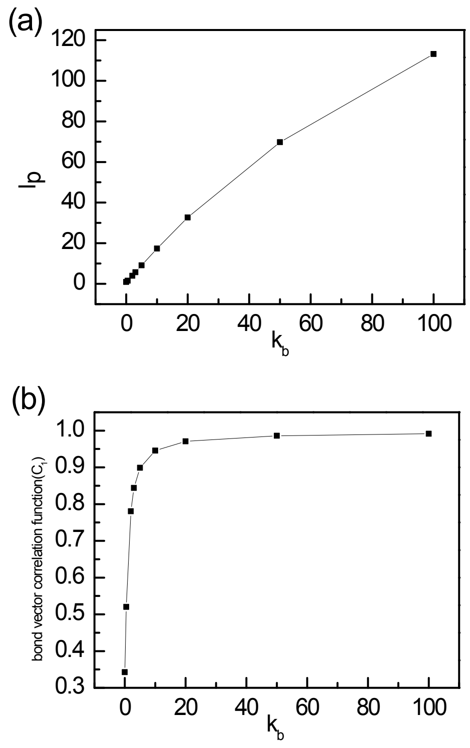

Fig.S2. (a) The persistence length, l_P, and (b) the bond vector correlation function, C_1, as a function of bending energy k_b for the central cyclic polymer.

b_i and b_{i+1} are the bond vectors of i-th and (i+1)-th beads of the central ring polymer. In fact, C_1=<cosθ'>, here $\theta'$is the angle between two adjacent bond vectors of central cyclic polymer. Fig. S2 shows the results for (a) persistence length l_P and (b) bond vector correlation function C_1, as a function of the bending energy k_b of the central ring polymer.

S3. The rotational diffusion of rigid central ring polymer

In order to analysis the rotational diffusion of the central cyclic polymer, we computed the time autocorrelation function $< \vec{u}(t) \cdot \vec{u}(0) >$ of a unit vector $\vec{u}(t)$ directed along the longest chain dimension. Here $\vec{u}(t)$ is taken to be along the diameter vector $\vec{u}_d(t) = \vec{u}_{N_L/2}(t)$ for the ring polymer[5]. We calculated the time autocorrelation function for the stiff central cyclic polymer with k_b=100, and the results are shown in Figure S3. Through a Kohlrausch-Williams-Watts (KWW) function of the form[5]:

$$< \vec{u}(t) \cdot \vec{u}(0) >= \exp[-(\frac{t}{\tau_{KWW}})^{\beta}] \qquad \text{(S3)}$$

where τ_{KWW} and β are the characteristic relaxation time and stretching parameter, respectively, we can calculate the relaxation time τ_{KWW} which is estimated from the reciprocal of the slope of corresponding curve in Figure S3. According to Table S1, with the ring size N_S increasing, the relaxation time τ_{KWW} decreases, which

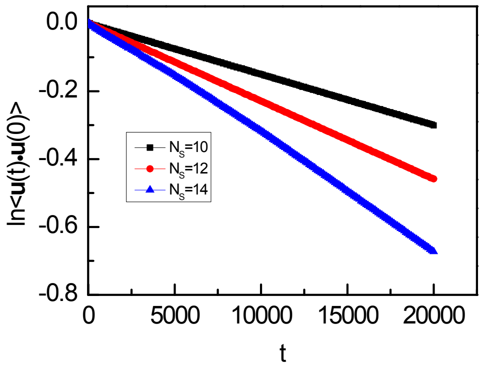

Fig.S3. The logarithm of the time autocorrelation function as a function of the time *t* for different ring size N_S. Here the bending energy of central ring polymer is k_b=100.

indicates that the central cyclic polymer shows a faster rotational diffusion for large N_S. These results also prove that the friction between the ring and central polymer is weakened as increasing small ring size.

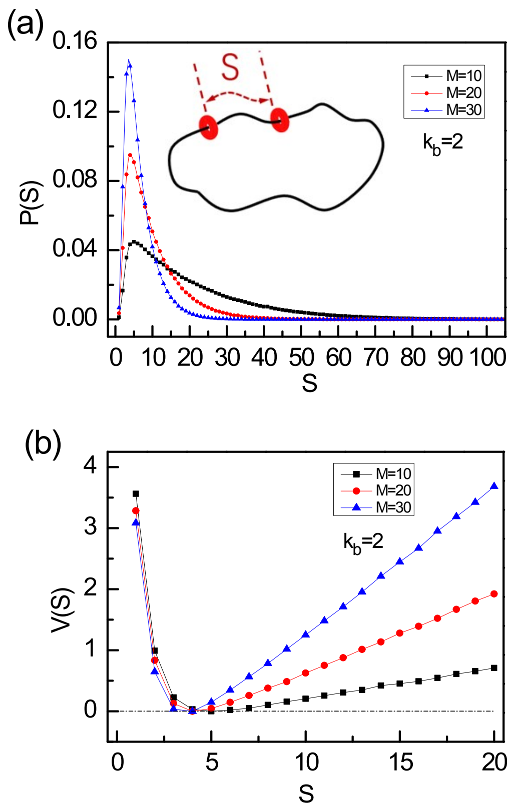

Fig. S4. (a)Probability distribution *P*(S) of two neighboring rings for different ring numbers *M* (b) Potential of mean force *V*(*S*) for small rings with k_b=2 for different *M*. Inset figure defines the path *S* between two neighboring rings.

Table S1. The relaxation time τ_{KWW} of rigid central cyclic polymer for different small ring sizes N_S.

N_S	10	12	14
τ_{KWW}	66500	43500	29700

S4. Potential of the mean force (PMF) V(S)

The probability distribution *P*(S) for rings along the central cyclic polymer is presented in Fig. S4(a), where *S* represents the path between two neighbouring rings, see the inset figure in Fig. S4(a). Here the rings don't penetrate each other during the whole simulation because there is the same size for all small rings. As the small rings in poly[*n*]catenane are marked in number order initially, *S* is defined as

$$S_m = \begin{cases} i_{m+1} - i_m, & i_{m+1} - i_m \geq 0 \\ N_L + (i_{m+1} - i_m), & i_{m+1} - i_m < 0 \end{cases} \qquad \text{(S4)}$$

Where i_m is the index number of the monomer of the polymer closest to the *m*-th ring, and $i_{M+1} = i_1$. Meanwhile, the peak value of *P*(S) is enhanced with increasing the ring number from *M*=10 to 20, and 30. The ring-ring potential of the mean force (PMF) can be calculated by $V(S) = -k_B T ln P(S)$,[6-8] which represents the ring-ring potential as a function of *S*. Here, we take the minima of the PMF as the reference states.

S5. Effects of the threading ring polymer on static properties of the central cyclic polymer

The static properties of the central cyclic polymer are evaluated for various numbers of the threading rings M. Figs. S5(a) and (b) show the mean-square radius of gyration, <$R_g{}^2$>, and the relative ratio of bond vector correlation function of the central ring polymer, $(C_1)_{M}/(C_1)_{M=0}$, for various bending energies k_b with different *M*, respectively. Here, the mean-square radius of gyration <$R_g{}^2$> is defined as $< R_g{}^2 >= \frac{1}{N_L} < \sum_{i=1}^{N_L} (r_i - r_{cm})^2 >$, where r_{cm}denotes the center-of-mass of the central polymer, N_L is the number of monomers in polymer. It is shown that the presence of the threading rings does not greatly affect the statistics properties of the central cyclic chain except for the flexible central ring polymer, i.e., $k_b < 2$.

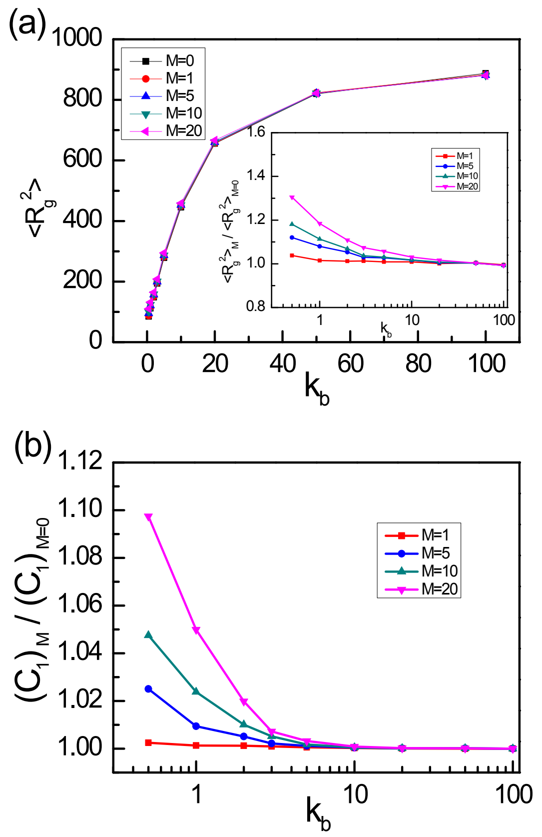

Fig. S5. (a) Mean square radius of gyration, <R_g^2> and (b) the relative ratio of $(C_1)_M/(C_1)_{M=0}$, as a function of bending energy k_b for different ring number M. Here the inset figure in Fig. S5(a) is the relative ratio of <R_g^2>$_M$/<R_g^2>$_{M=0}$, and N_S=10.

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