Supporting Information

Dynamics of a two-dimensional active polymer chain with a rotation-restricted active head

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1. Orientational autocorrelation function

The orientational autocorrelation function $C(t)$ of the orientation of self-propulsion force, $\mathbf{n}(t)$, is defined as $C(t) = \langle \mathbf{n}(t_0) \cdot \mathbf{n}(t + t_0) \rangle$. The evolution of $C(t)$ with time t is presented in Figure S1. We find that $C(t)$ roughly decays exponentially as $C(t) = e^{-t/\tau_r}$. Here the persistence time τ_r is estimated mostly from the decay of $C(t)$ in the region $0.05 < C(t) < 0.5$ where $C(t)$ shows the best exponential decay.
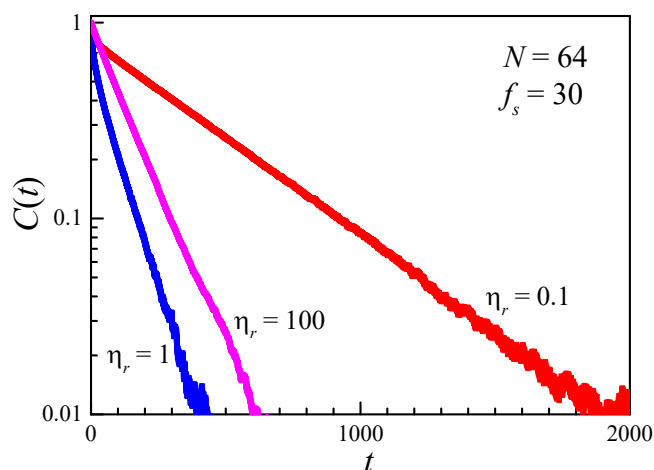
Fig. S1. Semi-logarithm plot of the evolution of the orientational autocorrelation function of the self-propulsion force, $C(t)$, for the active polymer with a rotation-restricted head ABP. Polymer length $N = 64$ and self-propulsion force $f_s = 30$.

2. Elongation of the active polymer chain with a rotation-restricted head ABP

Figure S2 presents the dependence of the mean square radius of gyration $<R_G^2>$ on the rotational friction coefficient η_r for polymer chains of length $N = 64$ under self-propulsion force $f_s = 7$ and 30. We can see that $<R_G^2>$ of the active polymer under self-propulsion is always larger than that of a corresponding passive polymer ($f_s = 0$) with $<R^2>_0 = 69 \pm 2$ for $N = 64$.

Figure S3 presents the dependence of mean square end-to-end distance $<R^2>$ and $<R_G^2>$ on self-propulsion force f_s. $<R^2>$ and $<R_G^2>$ increase gradually with increasing f_s.

Figure S4 presents the dependence of $<R^2>$ and $<R_G^2>$ on N for the active polymer with $f_s = 30$ and the corresponding passive polymer ($f_s = 0$). For the passive polymer, we have $<R^2> \propto N^{1.5}$ and $<R_G^2> \propto N^{1.5}$. The exponent 1.5 is consistent with the known result for two-dimensional self-avoiding polymers. While for the active polymer with $f_s = 30$, we find the scaling exponent is close to 2 for relatively short chains, indicating a rod-like conformation under self-propulsion of the head ABP. We find the data deviate gradually from the scaling relations $<R^2> \propto N^2$ and $<R_G^2> \propto N^2$ with the increase of N. And $<R^2>$ and $<R_G^2>$ of long RRAP tend to approach that of the passive polymer. The reason is that the effect of the self-propulsion of the head ABP is limited, i.e., the RRAP becomes flexible with increasing N.
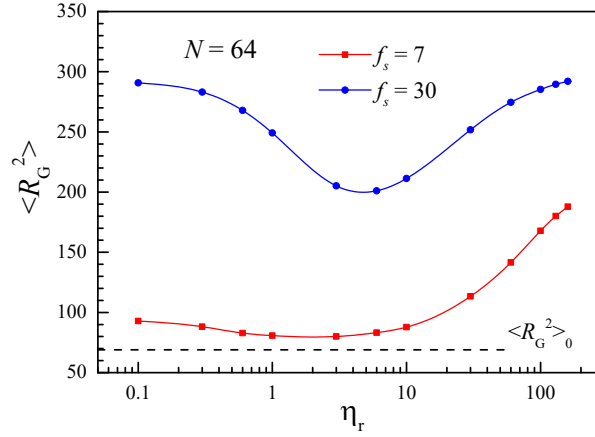
Fig. S2. Log-log plot of the mean square radius of gyration $<R_G^2>$ versus the rotational friction coefficients η_r for the active polymer of length $N = 64$ under self-propulsion force $f_s = 7$ and 30. The dashed line with $<R_G^2>_0 = 69 \pm 2$ denotes $<R_G^2>$ of the corresponding passive polymer chain of $N = 64$.
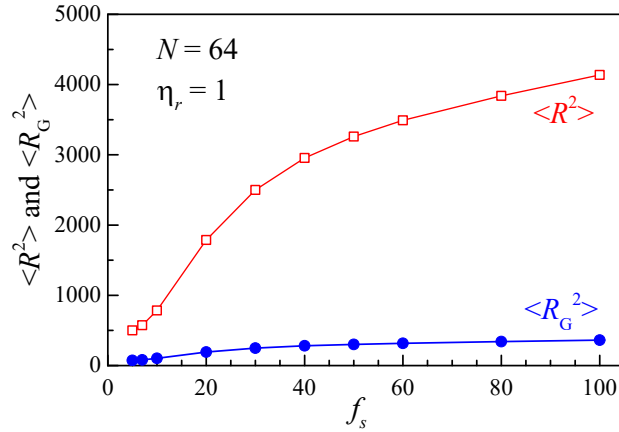
Fig. S3. Plot of mean square end-to-end distance $<R^2>$ and mean square radius of gyration $<R_G^2>$ versus self-propulsion force f_s for the active polymer. Polymer length $N = 64$ and rotational friction coefficient $\eta_r = 1$.
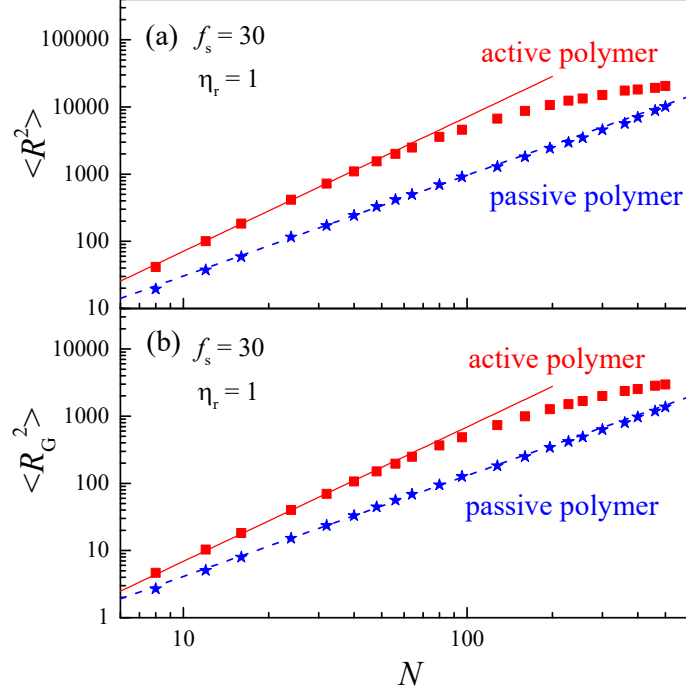
Fig. S4. Log-log plot of mean square end-to-end distance $<R^2>$ (a) and mean square radius of gyration $<R_G^2>$ (b) versus polymer length N for the active polymer (red squares) with $f_s = 30$ and the corresponding passive polymer (blue stars). The rotational friction coefficient is $\eta_r = 1$. The red solid lines have a slope of 2 and the blue dashed lines have a slope of 1.5.

3. Diffusion property

The mean squared displacement of the two-dimensional active polymer at long timescales can be expressed as $<\Delta r^2(t)> = 4D_{eff}t$. The diffusion of the active polymer can be attributed to the active force of ABP and thermal noise. Thus we have $D_{eff} = D_P + D_T$ with D_P and D_T are the coefficients of propulsive and thermal diffusion, respectively. For the present active polymer model, we have $D_P \propto f_s^2\tau_r/N^2\eta_t^2$ and $D_T \propto k_BT/N\eta_t$. It is interesting to estimate the crossover value of $f_{s,c}$ at which $D_P = D_T$. We thus have a simple relation $f_{s,c}^2 \propto k_BT\eta_tN/\tau_r$.
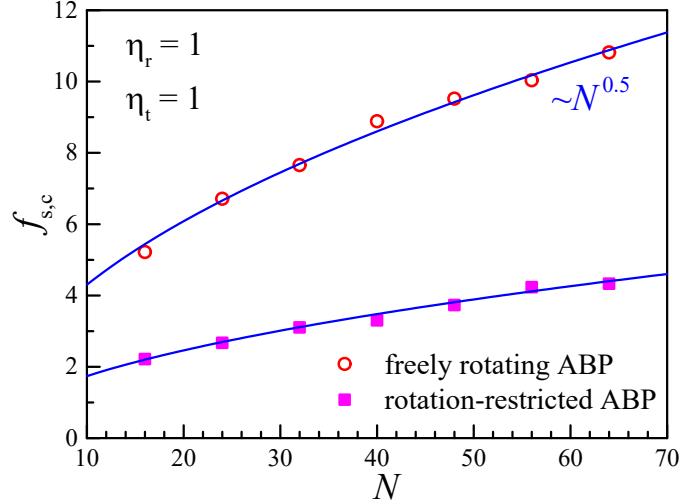
Fig. S5. Plot of the crossover value of $f_{s,c}$ versus polymer length N for the active polymer with a rotation-restricted head ABP (with **M**) and that with a freely rotating head ABP (**M** = 0). Solid lines show the relation $f_{s,c} \propto N^{0.5}$.

We have checked the dependence of $f_{s,c}$ on N for $\eta_t = 1$ and $\eta_r = 1$. The simulation results are presented in Figure S5 for the active polymer with a rotation-restricted head ABP (with **M**) and that with a freely rotating head ABP (**M** = 0). We find $f_{s,c}$ is small for the active polymer with a rotation-restricted head ABP, in agreement with that the restriction of rotation of the head ABP will enhance the diffusion. It is interesting to see that $f_{s,c} \propto N^{0.5}$ still holds for the active polymer with a rotation-restricted head ABP. The reason may be that, for the active polymer with **M**, the variation of $f_{s,c}$ is very small, so that τ_r can be regarded as a constant independent of f_s and N. The influence of N on τ_r is rather weak at small f_s since the deformation of polymer is small at small f_s.