Supporting Information

Knotting and adsorption of end-grafted active polymers

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1. Supplementary Plots

1.1. Active polymer model

The active polymer is composed of an active head and a subsequent end-grafted passive polymer block. This kind of active polymer model might capture the main characteristics of biopolymers with local activity. Some biopolymers, like spermatozoa, bacilli, and spirochetes, move with the help of local active parties of their bodies [L. Natali, L. Caprini and F. Cecconi, How a local active force modifies the structural properties of polymers, *Soft Matter*, 2020, **16**, 2594–2604.]. The active head is represented by a Janus particle as shown in Figure S1. The passive polymer is connected to the edge of the active head opposite to the direction of the active force F_a. The FENE force, F_{FENE}, acting on the active head does not point toward the center of mass of the active head, so it creates a torque $M = R \times F_{FENE}$ on the active head and restricts the rotation of the active head.
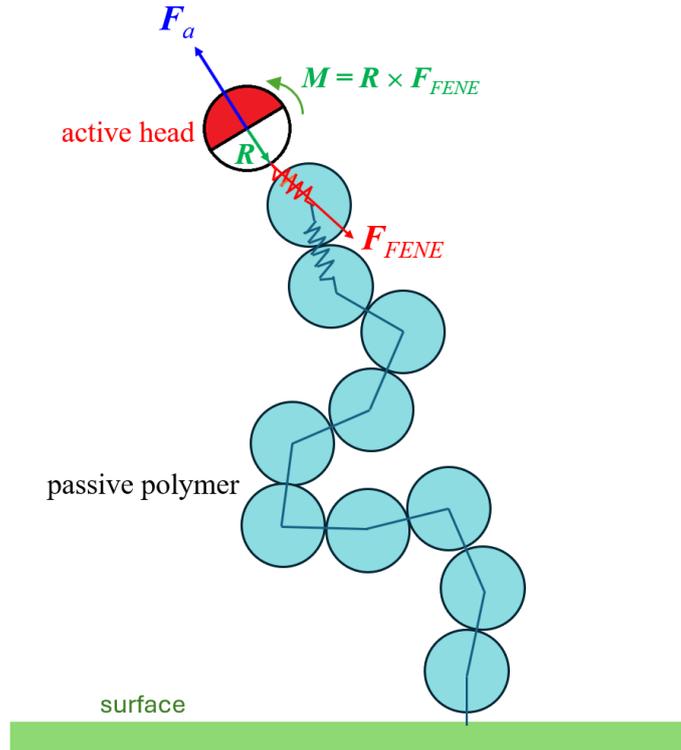
Figure S1. A sketch of the active polymer end-grafted on a surface. The active head of the active polymer is represented by a Janus particle. The first bond connecting the active and passive beads is different from the other bonds connecting two passive beads. When the FENE force of the first bond does not pass through the center of the active head, the active head is subjected to a torque M.

1.2. Method to determine knot in a polymer chain

It is of significant challenge to ascertain whether knots exist within polymer chains through mathematical means. In this work, we use the simulation method to figure out the knots. To this end, we exerted a sufficiently large artificial stretching force on the active head of the polymer, which was directed vertically outward from the surface. An unknotted polymer is likely to be stretched to its fullest extent (Figure S2c), while a knotted one will resist such complete elongation (Figure S2b). Consequently, we can accurately distinguish between a knotted polymer and an unknotted one.
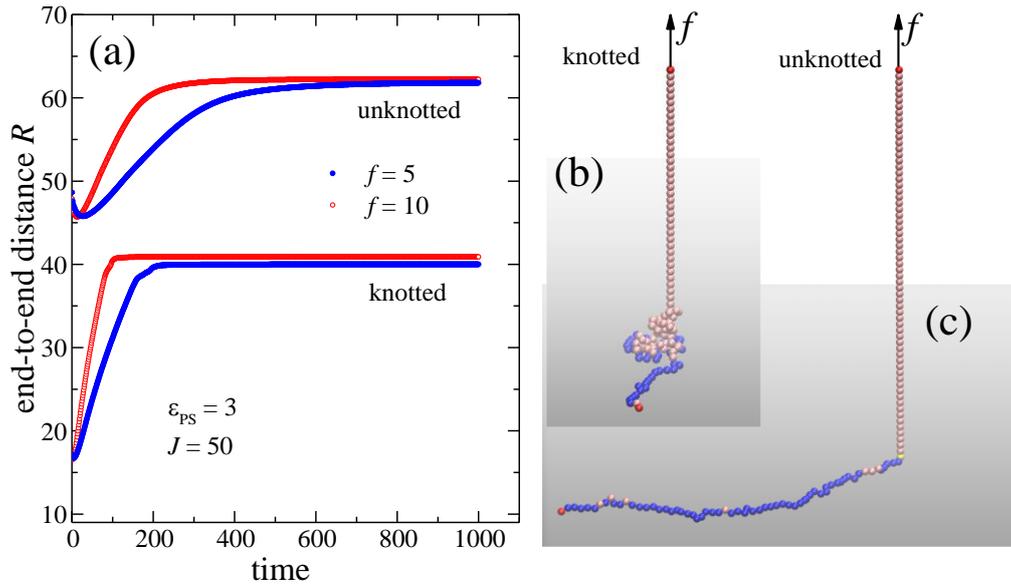
Figure S2. (a) Evolution of end-to-end distance R with time when a stretching force f is applied starting from $t = 0$. (b) and (c) plot the knotted polymer and unknotted polymer, respectively. The polymer conformations before and after applying the stretching force f are plotted in the same plane. Red, tan, blue, and pink beads represent the active head, grafted bead, adsorbed beads, and non-adsorbed beads, respectively.

Figure S2a shows that the evolution from an adsorbed polymer to a stretched one is fast. The results are roughly independent of the magnitude of the stretching force f if it is sufficiently large.

1.3 Knotted region in the active polymer

The probability that a bead is part of a knotted region is calculated from the KymoKnot software package [L. Tubiana, G. Polles, E. Orlandini and C. Micheletti, Kymoknot: A web server and software package to identify and locate knots in trajectories of linear or circular polymers. *Euro. Phys. J. E*, 2018, **41**, 72]. KymoKnot software package can give the position of the knot in the polymer chain. The results are plotted in Figure S3 for the active polymer of length $N = 65$ with the active force $F_a = 5$. We find that knots appear close to the grafted end for both $J = 0.1$ and 50.
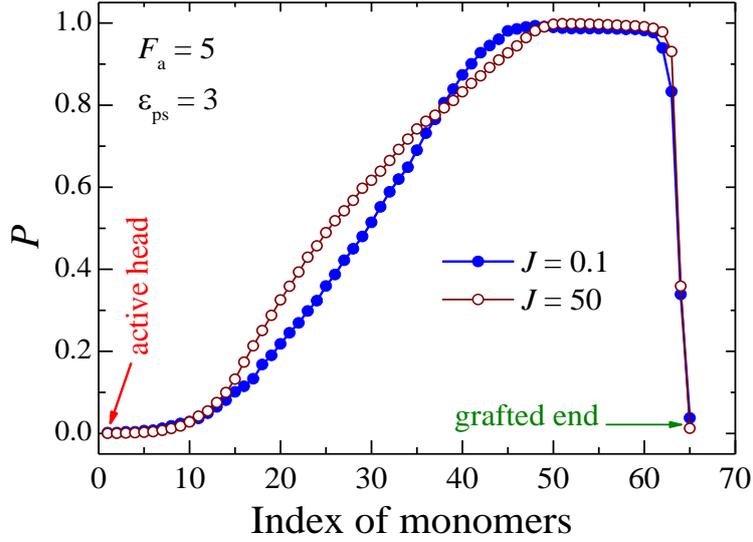
Figure S3. Plot of the probability that a bead is part of a knotted region. The active head is indexed 1 and the grafted end is indexed N. Polymer length $N = 65$ and the active force $F_a = 5$.

1.4 Relation between knotting and adsorption

The adsorption of the active polymer chain is mainly dependent on the attraction strength of the surface ε_{PS} and the active force F_a. Knots in polymer chains play a relatively weak role. To show the relation between knotting and adsorption, we perform a simulation by varying J while $\varepsilon_{PS} = 1.5$ and $F_a = 5$ are kept constant. We know that knotting is discouraged by decreasing the value J. Starting from the steady state obtained at $J = 50$, we continued the simulation after changing J to 0.1 at $t = 0$. The simulation results are shown in Figure S4. We can see that the probability of knotted polymer (P_{knot}) decreases while the number of adsorbed monomers ($<M>$) increases over time. The result indicates that the knotting in the active polymer hinders the adsorption.
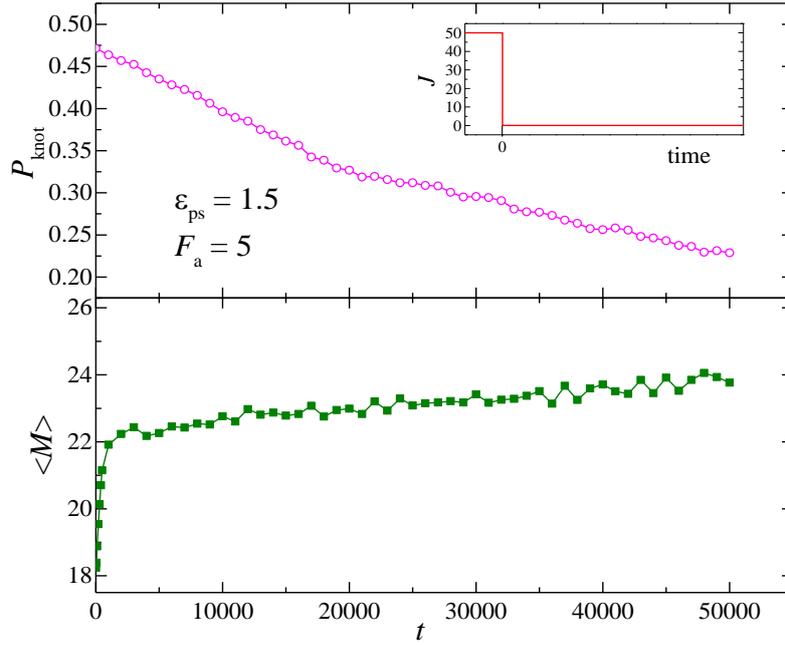
Figure S4. Evolution of the probability of knotted polymers P_{knot} (a) and the mean number of adsorbed monomers $<M>$ (b) when the rotational inertia J is suddenly decreased from 50 to 0.1 for the active polymer of length $N = 65$. Other parameters: the attraction strength of the surface $\varepsilon_{PS} = 1.5$ and the active force $F_a = 5$.

1.5 Dynamical orientational correlation function

Figure 9 in the manuscript presents the variation of the dynamical orientational correlation function $C(t)$ versus time t in the semi-logarithm scale. The double-logarithmic plot of Figure 9 is presented in Figure S5. The log-log behavior emerges at the moderate range of the simulation time.
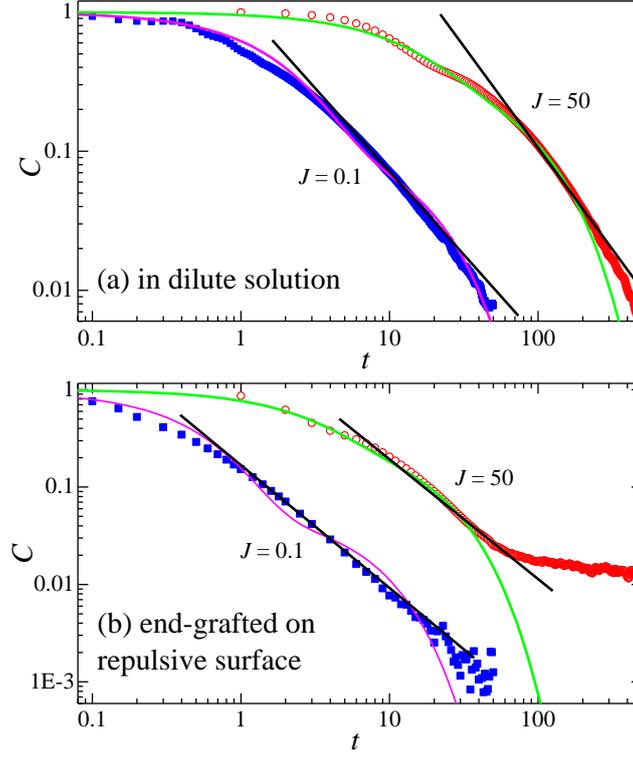
Figure S5. Log-log plot of the dynamical orientational correlation function $C(t)$ versus time t for free active polymer chains in the dilute solution (a) end-grafted active polymers on a repulsive surface (b). Polymer length $N = 65$, rotational inertia $J = 0.1$ and 50, and active force $F_a = 5$. Straight lines are guides for the eyes.

1.6 Relaxation time

The relaxation time of the end-to-end vector of a free polymer chain in a dilute solution is evaluated from the self-correlation function of the end-to-end vector R, $C_R(t) = <R(t_0) \cdot R(t + t_0)>/<R^2>$. Figure S6 plots the variation of $C_R(t)$ versus time t for a free polymer chain of length $N = 65$. From the exponential decay function $C_R(t) = e^{-\frac{t}{\tau_R}}$, we estimate τ_R is about $630\tau_0$.
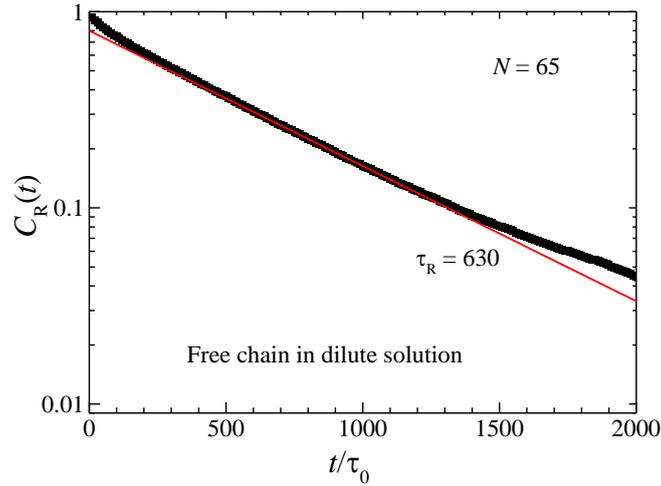
Figure S6. Semi-logarithm plot of the self-correlation function of the end-to-end vector, $C_R(t)$ versus time t for a free polymer chain of length $N = 65$ in the dilute solution. The straight line with $\tau_R = 630$ is a guide for the eyes.

2. Original simulation data
2.1. Figure 3

J	$N = 33$		$N = 65$	
	ε_{PS}^{*}	error	ε_{PS}^{*}	error
0.1	1.4	0.02	1.17	0.02
0.2			1.17	0.02
0.5			1.17	0.02
1	1.45	0.02	1.18	0.03
2	1.5	0.02	1.22	0.03
5	1.52	0.03	1.25	0.03
10	1.55	0.03	1.28	0.03
15	1.55	0.05		
20	1.57	0.05	1.34	0.05
30	1.58	0.05	1.37	0.05
50	1.62	0.05	1.45	0.05

J	$N = 33$		$N = 65$	
	φ^{*}	error	φ^{*}	error
0.1	0.309	0.01	0.238	0.01
0.2			0.235	0.01
0.5			0.229	0.01
1	0.31	0.01	0.229	0.01
2	0.317	0.01	0.235	0.01
5	0.315	0.01	0.234	0.01

10	0.318	0.01	0.232	0.01
15	0.315	0.01		
20	0.321	0.01	0.24	0.01
30	0.321	0.015	0.248	0.015
50	0.336	0.015	0.266	0.015

2.2 Figure 6

J	P_{knot}	$<M>$ of unknotted polymers	$<M>$ of knotted polymers
0.1	0.254	48.43	40.61
0.2	0.234	48.44	40.40
0.5	0.224	48.30	39.99
1	0.304	48.27	39.51
2	0.402	48.32	38.91
5	0.534	48.46	37.54
10	0.663	48.55	36.61
20	0.735	48.77	36.19
30	0.743	48.87	36.90
50	0.766	49.12	37.29

2.3 other figures

Data of other figures are too large to be included here. Data of other figures (file name: data_of_Figures.zip) can be downloaded at the website：

https://zjuem.zju.edu.cn/coremail/common/nfFile.jsp?share_link=6F569F2CE26D4E F6B6C23C080FF7B61B&uid=luomengbo%40zju.edu.cn
with password: MJ64

3. Codes

The Langevin dynamics simulation codes (file name: active_polymer_adsorption.zip) for the present manuscript can be downloaded at the website：

https://zjuem.zju.edu.cn/coremail/common/nfFile.jsp?share_link=B79B47AC7E134C 54BEC675F36567AD02&uid=luomengbo%40zju.edu.cn
with password: X3vT