

Electronic Supplementary Information

Adsorption of active polymers on attractive nanoparticles

Yi-Fan Shen, Han-Xian Hu, and Meng-Bo Luo*

School of Physics, Zhejiang University, Hangzhou 310027, China.

Corresponding Author

* Meng-Bo Luo (luomengbo@zju.edu.cn)

1. Adsorption of polymer chain during the annealing process

We increase the nanoparticle's attraction strength (ε_{pn}) slowly from below the critical adsorption point ε_{pn}^* to above ε_{pn}^* . While the polymer chain changes from a desorbed state at low ε_{pn} to an adsorbed state at high ε_{pn} . The nanoparticle's attraction strength ε_{pn} is the main parameter that changes the adsorption state of polymer chains. Here polymer length is $N = 64$ and nanoparticle size is $\sigma_{NP} = 5$. Figure S1 shows some typical snapshots of the polymer chain at different ε_{pn} during the annealing process for an active force $F_a = 10$ on the head ABP. It was found ε_{pn}^* is about 3.2. We can see adsorption around and above ε_{pn}^* .

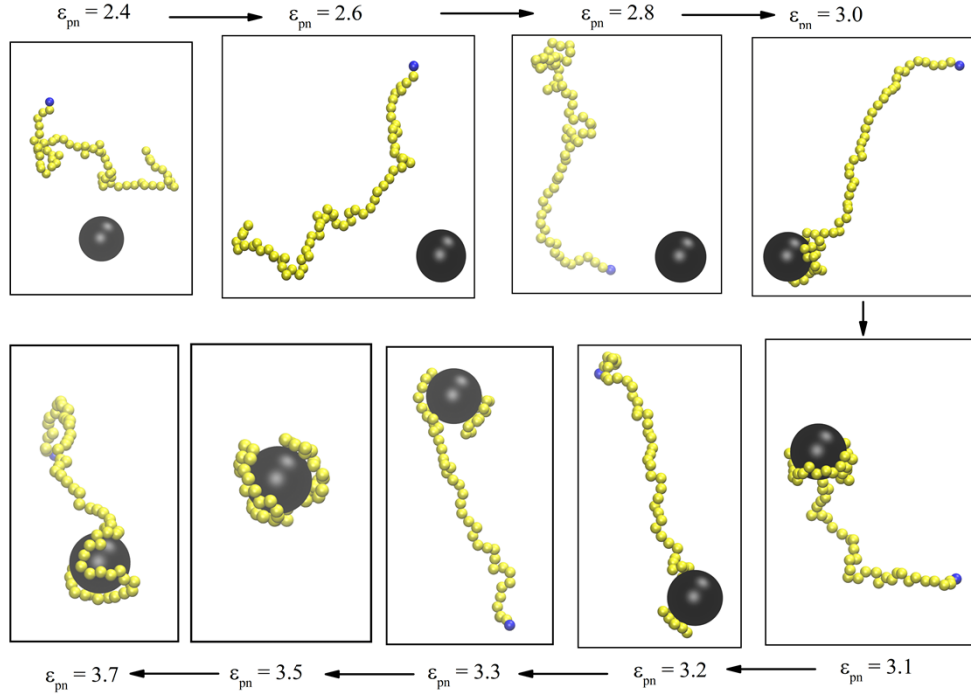


Figure S1. Snapshots of polymer for different nanoparticle interaction strength ϵ_{pn} . Chain length $N = 64$, active force $F_a = 10$, and nanoparticle size $\sigma_{NP} = 5$.

2. Relation between the number of adsorbed monomers and the length of the tail

For the adsorbed active polymer chains, both the number of adsorbed monomers and the length of the tail near the head ABP are dependent on the active force F_a on the head ABP. Figure S2 shows the variation of the mean number of adsorbed monomers $\langle n_a \rangle$ with the mean length of the tail near the head ABP $\langle L_{tail} \rangle$ for polymer length $N = 64$ and the nanoparticle's attraction strength $\epsilon_{pn} = 4$. The size of the nanoparticle is $\sigma_{NP} = 5$. We find $\langle n_a \rangle$ decreases roughly linearly with an increase in $\langle L_{tail} \rangle$.

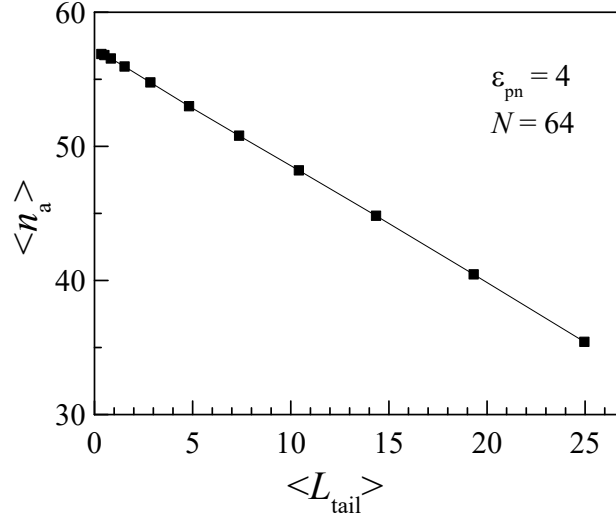


Figure S2. Plot of the mean number of adsorbed monomers $\langle n_a \rangle$ versus the mean length of the tail near the head ABP $\langle L_{\text{tail}} \rangle$ for the adsorbed active polymer chains. Polymer length $N = 64$ and nanoparticle's attraction strength $\varepsilon_{\text{pn}} = 4$.

3. Kinetics of monomers in active polymer chains

We have calculated the mean squared velocity, $\langle v^2 \rangle$, of the monomers in the adsorbed active polymers. Figure S3 shows the results for RRAP chains with active forces $F_a = 0, 5, \text{ and } 10$. For $F_a = 0$ case, the value of $\langle v^2 \rangle = 3$ is consistent with the temperature T

$= 1$, according to the energy equalization theorem $\frac{1}{2}mv^2 = \frac{3}{2}k_B T$. Here the mass of the

polymer monomer is set as unity and $k_B = 1$ as all quantities are dimensionless in the simulations. When the active force is considered, the value of $\langle v^2 \rangle$ is increased for the monomers close to the head ABP (monomer index 1). The results show that monomers near the ABP experience a higher effective temperature.

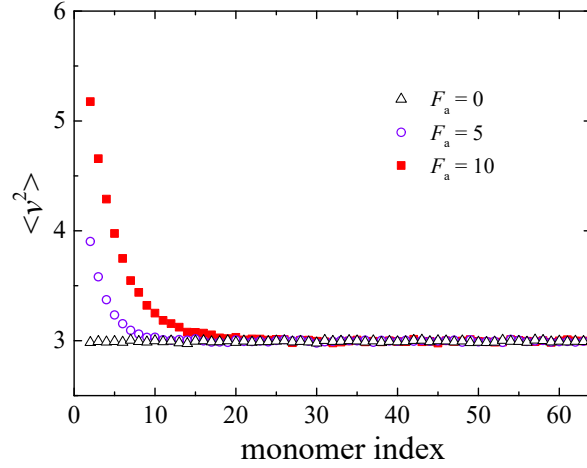


Figure S3. Plot of the mean squared velocity of the passive monomers in the adsorbed polymers. Polymer length $N = 64$ and nanoparticle's attraction strength $\epsilon_{pn} = 4$.

4. Simulation results for FRAP chain

Figure S4 presents some simulation results of the FRAP chain of polymer length $N = 64$. The size of the nanoparticle is $\sigma_{NP} = 5$. Adsorption probability $P(n_a)$, mean number of adsorbed monomers $\langle n_a \rangle$, and the fluctuation of the number of adsorbed monomers $\langle \delta n_a^2 \rangle$ are plotted for the FRAP chain with an active force $F_a = 10$ and the corresponding passive polymer ($F_a = 0$). From the fluctuations of the number of adsorbed monomers $\langle \delta n_a^2 \rangle$, the critical adsorption point ϵ_{pn}^* is estimated.

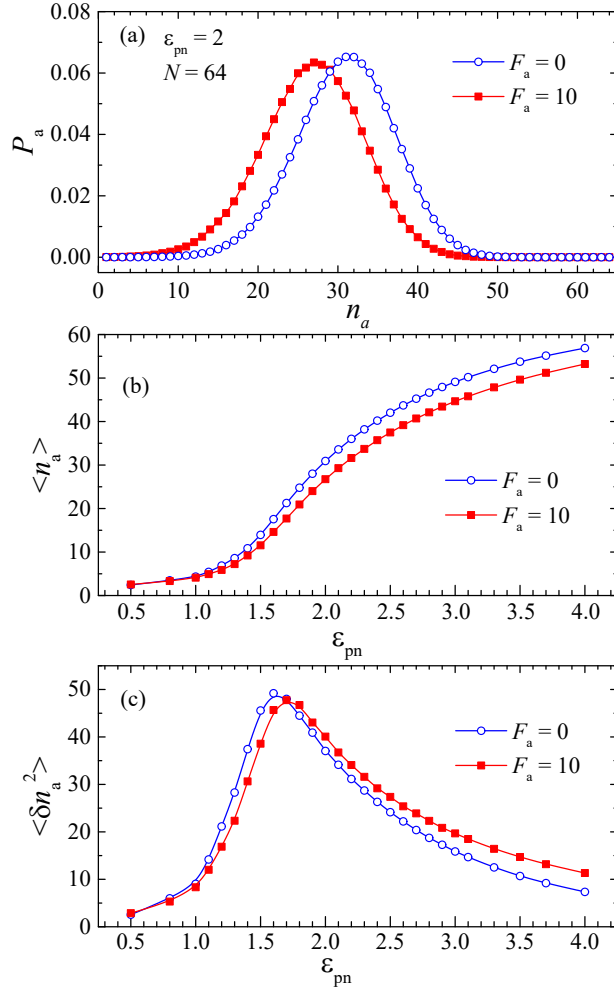


Figure S4. (a) Plot of the adsorption probability $P(n_a)$ versus the number of adsorbed monomers n_a for a passive polymer ($F_a = 0$) and a FRAP with an active force $F_a = 10$; (b) Plot of the mean number of adsorbed monomers $\langle n_a \rangle$ versus the polymer-NP interaction strength; (c) The dependence of the fluctuation of the number of polymer-NP contacts $\langle \delta n_a^2 \rangle$ on the interaction strength ϵ_{pn} . The polymer length is $N = 64$.