Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Influence of various nanoparticle shapes on the interfacial chain mobility: A molecular dynamics simulation

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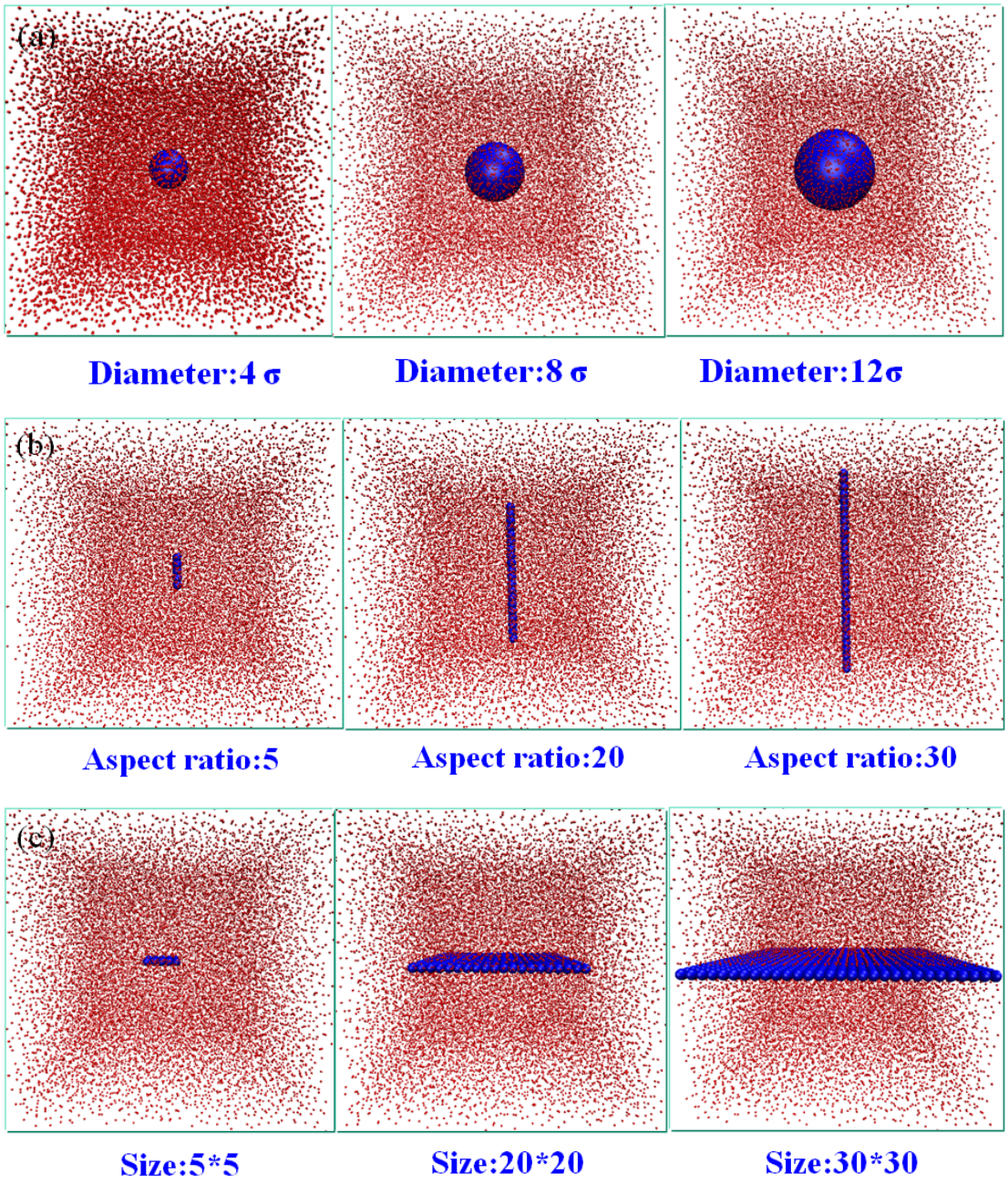
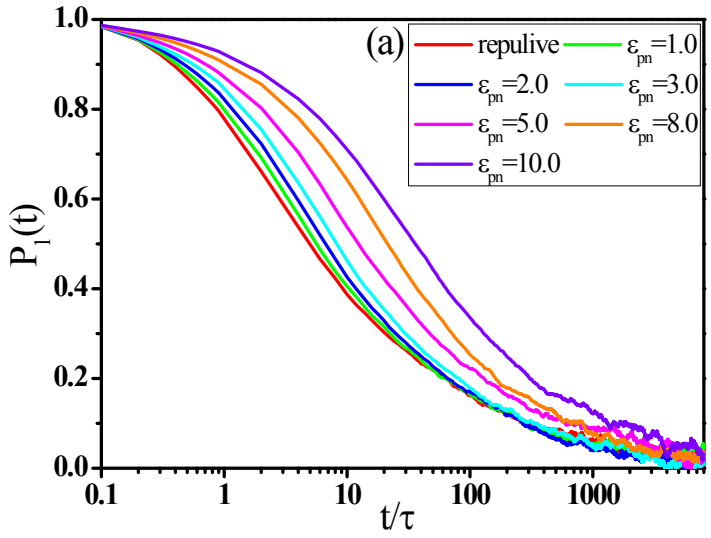
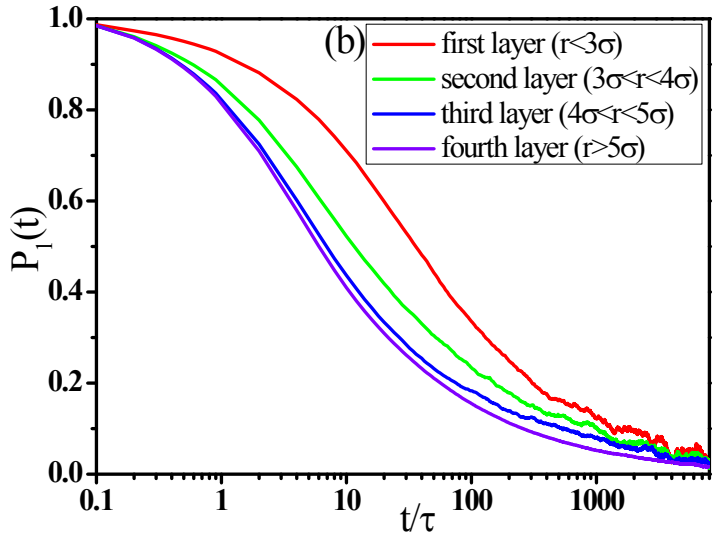


Fig. S1. Some snapshots of initial state for(a) nanosphere, (b) nanorod, (c) nanosheet.


(a)
repulive
ε_pn=1.0
ε_pn=2.0
ε_pn=3.0
ε_pn=5.0
ε_pn=8.0
ε_pn=10.0
P_1(t)
t/τ
0.0
0.2
0.4
0.6
0.8
1.0
0.1
1
10
100
1000


(b)
first layer (r<3σ)
second layer (3σ<r<4σ)
third layer (4σ<r<5σ)
fourth layer (r>5σ)
P_1(t)
t/τ
0.0
0.2
0.4
0.6
0.8
1.0
0.1
1
10
100
1000

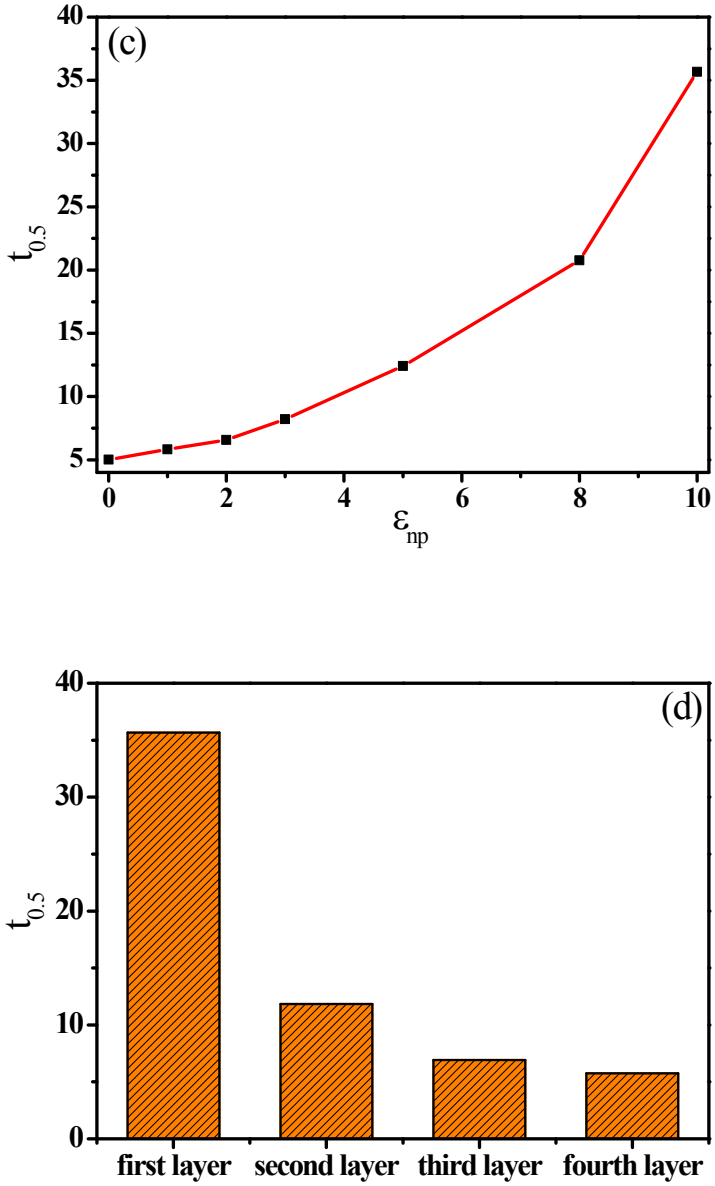


Fig. S2. The decay of the bond-orientation function $P_1(t)$ (a) in the L1 layers for different interfacial strength and (b) in different layers in the case $\varepsilon_{pn} = 10.0$. The characteristic relaxation time $t_{0.5}$ (c) for different polymer-nanoparticle interactions ε_{pn} and (d) for different layers.

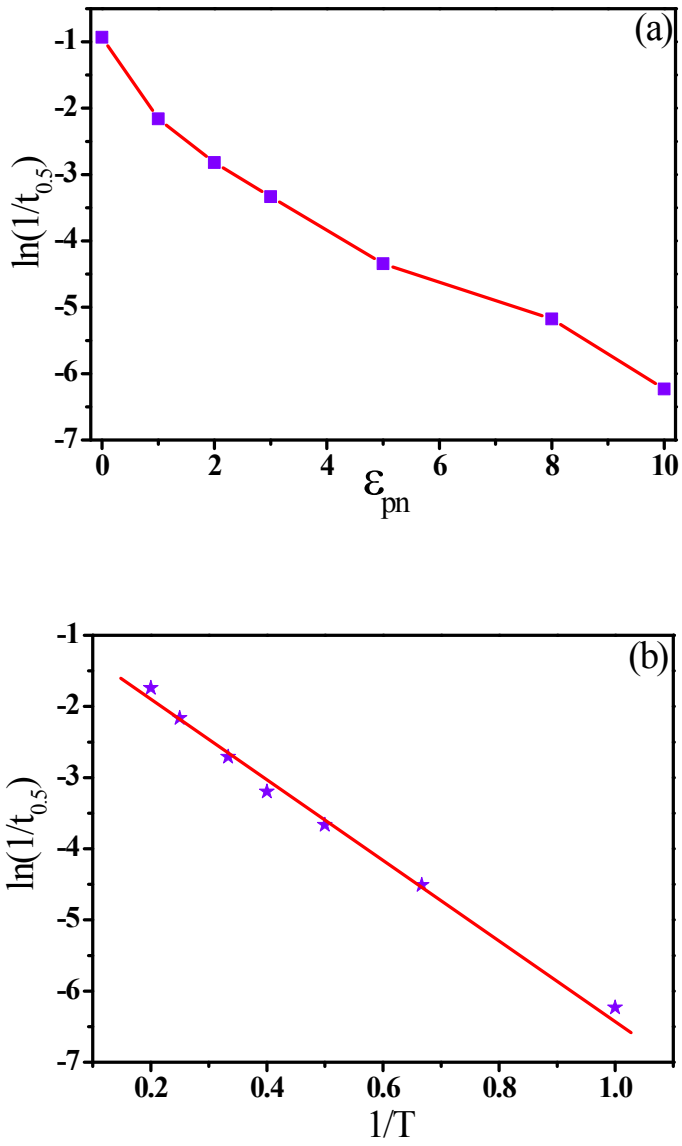


Figure S3. Logarithm of the desorption rate (the inverse of the desorption time $t_{0.5}$) (a) as a function of the polymer-nanoparticle interaction ε_{pn}. (b) as a function of the inverse of the temperature.

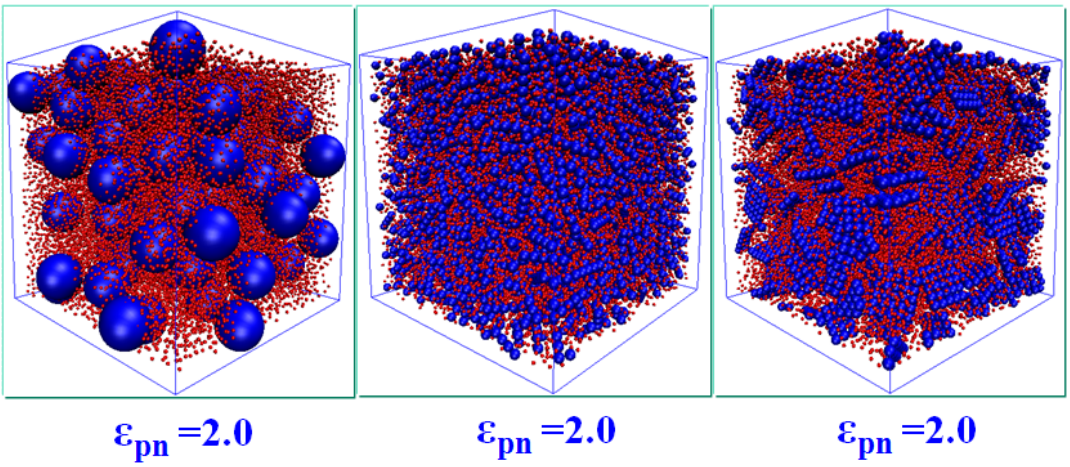


Fig. S4. Snapshots of one system ($\varepsilon_{pn} = 2.0$) (a) for nanosphere filled systems. (b) for nanorod filled systems. (c) for nanosheet filled systems.

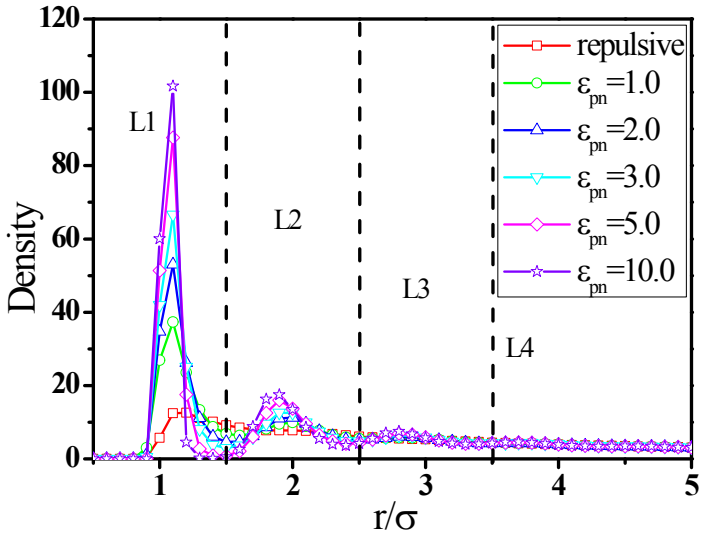


Fig. S5. Density profiles of polymer beads around the nanorod for several interfacial strengths;

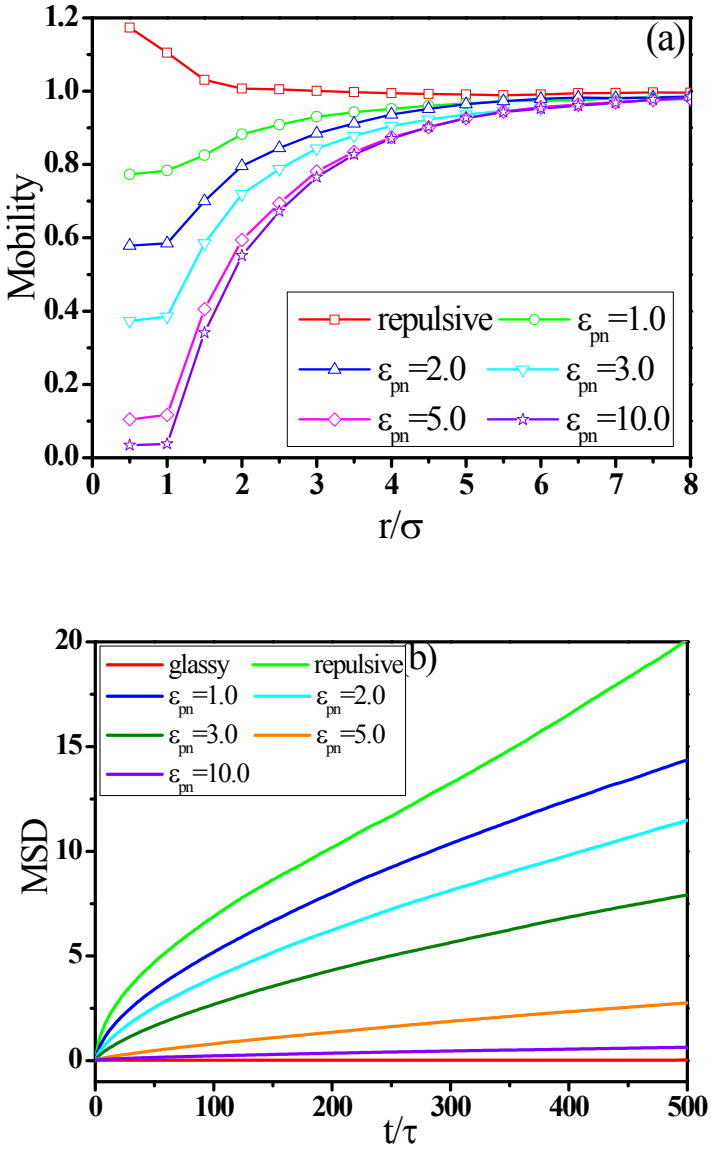


Fig. S6. (a) Mobility of the polymer beads as a function of the distance from the center of nanorod for different polymer-nanorod interactions. (b) Mean square displacement (MSD) averaging for polymer beads in the L1 region. For comparison, the MSD of polymer beads in the glassy state ($T<T_g$) is also shown.

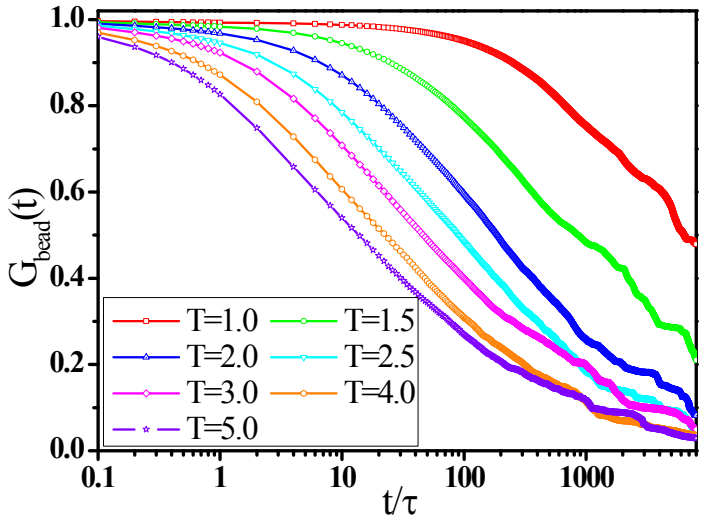


Fig. S7. Decay of $G_{bead}(t)$ for different temperatures in the case $\varepsilon_{pn} = 10.0$.

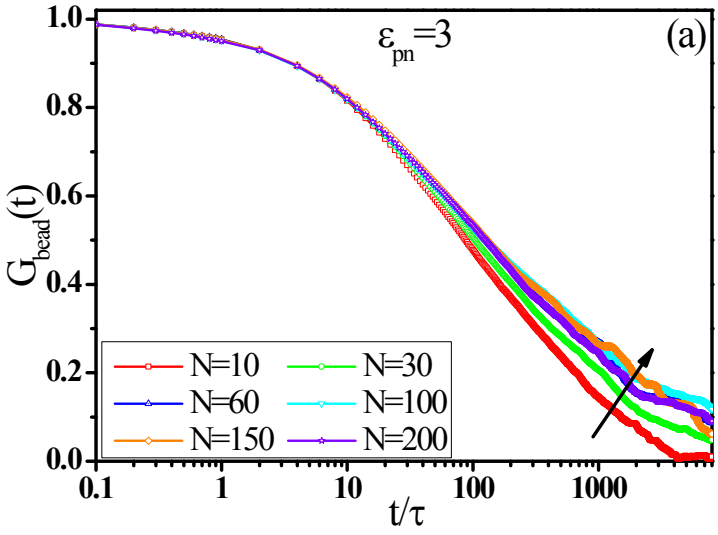


Fig. S8. Decay of $G_{bead}(t)$ for different chain lengths in the case $\varepsilon_{pn} = 3.0$.

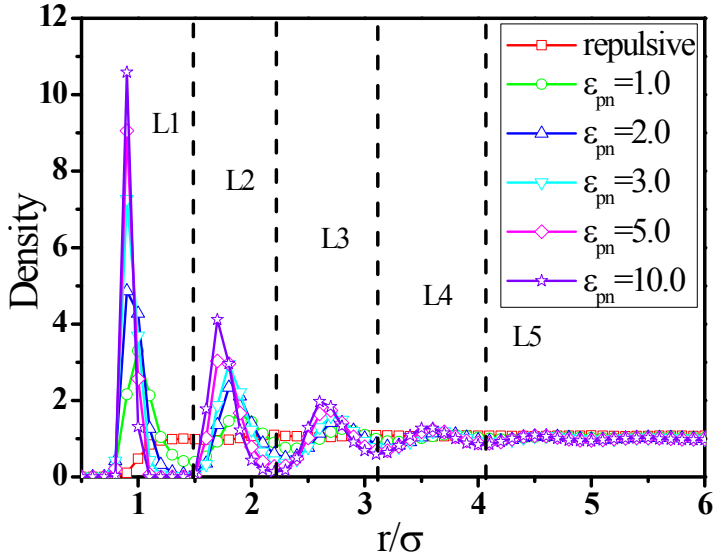
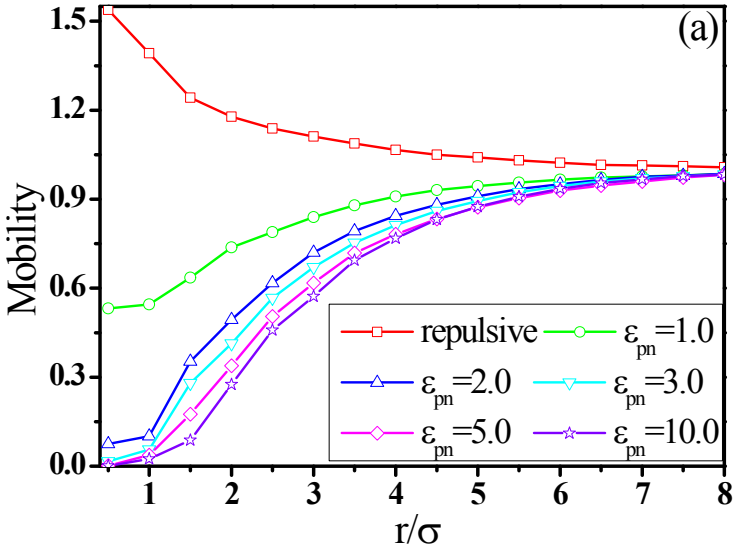


Fig. S9. Density profiles of polymer beads around the nanosheet for several interfacial strengths;



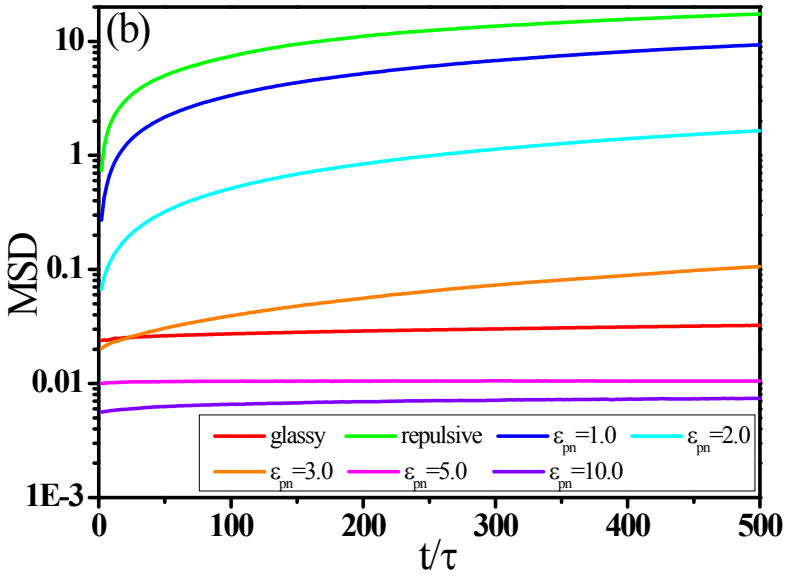


Fig. S10. (a) Mobility of the polymer beads as a function of the distance from the center of nanosheet for different polymer-nanosheet interactions. (b) Mean square displacement (MSD) averaging for polymer beads in the L1 region. For comparison, the MSD of polymer beads in the glassy state ($T<T_g$) is also shown.

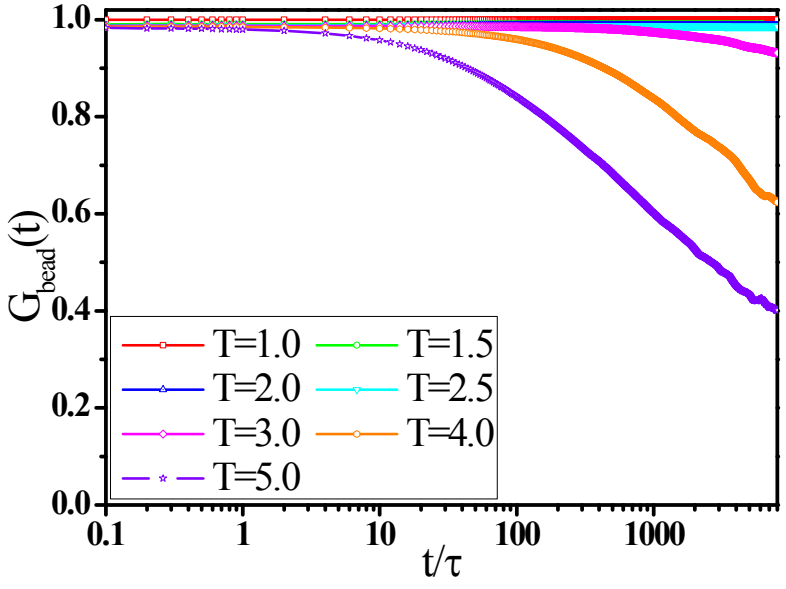


Fig. S11. Decay of $G_{bead}(t)$ for different temperatures at $\varepsilon_{pn} = 10.0$.

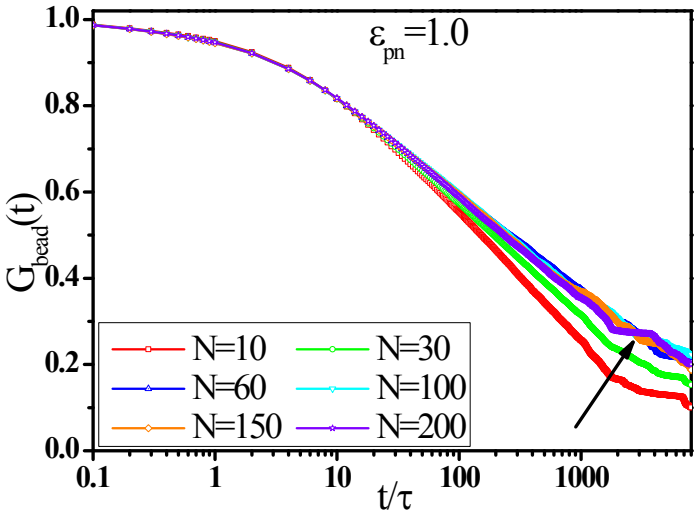


Fig. S12. Decay of $G_{bead}(t)$ for different chain lengths in the case $\varepsilon_{pn} = 1.0$.

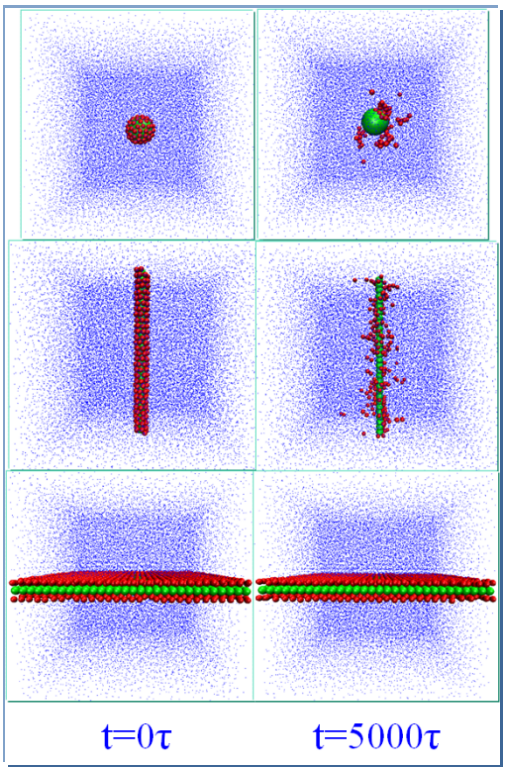


Fig. S13. The snapshots for the kinds of filler filled systems at time $t = 0\tau$ and $t = 5000\tau$. The red spheres denote the interfacial beads, the green beads denote the filler and the blue points denote other polymer. Note $\varepsilon_{pn} = 10.0$ here.

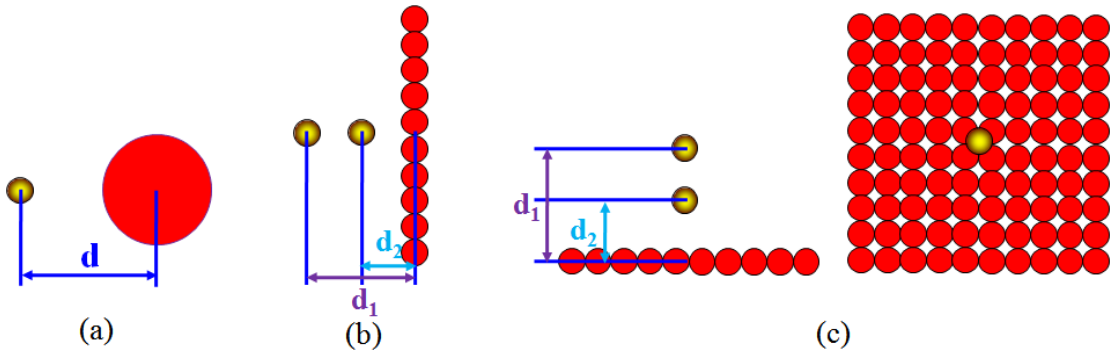


Fig. S14. (a) The red sphere denotes the nanoparticle, the yellow bead denotes polymer monomer and the d denotes the distance between the polymer bead and nanoparticle center; (b) The red spheres denotes the nanorod, the yellow beads denote polymer monomers and the d1 and d2 denote the distance between the polymer beads and nanorod center; (c) The red spheres denotes the nanosheet, the yellow beads denote polymer monomers and the d1 and d2 denote the distance between the polymer beads and nanosheet center; The left graph is viewed from the side and the right graph is viewed from the top.

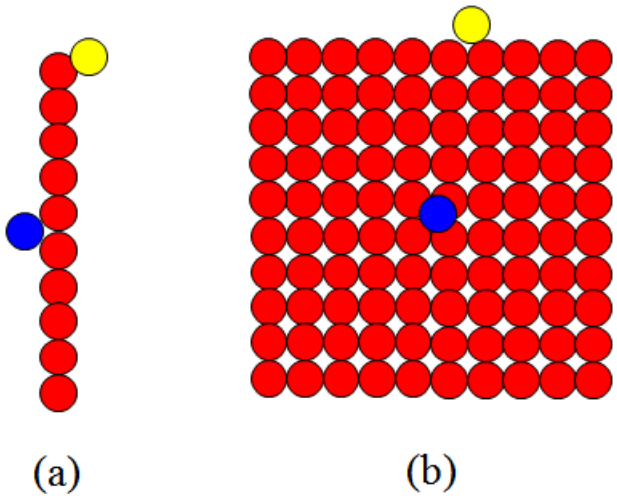


Fig. S15. (a) The red spheres denote the nanorod, the yellow bead and the blue bead denote polymer beads; (b) The red spheres denote the nanosheet, the yellow bead and the blue bead denote polymer beads.

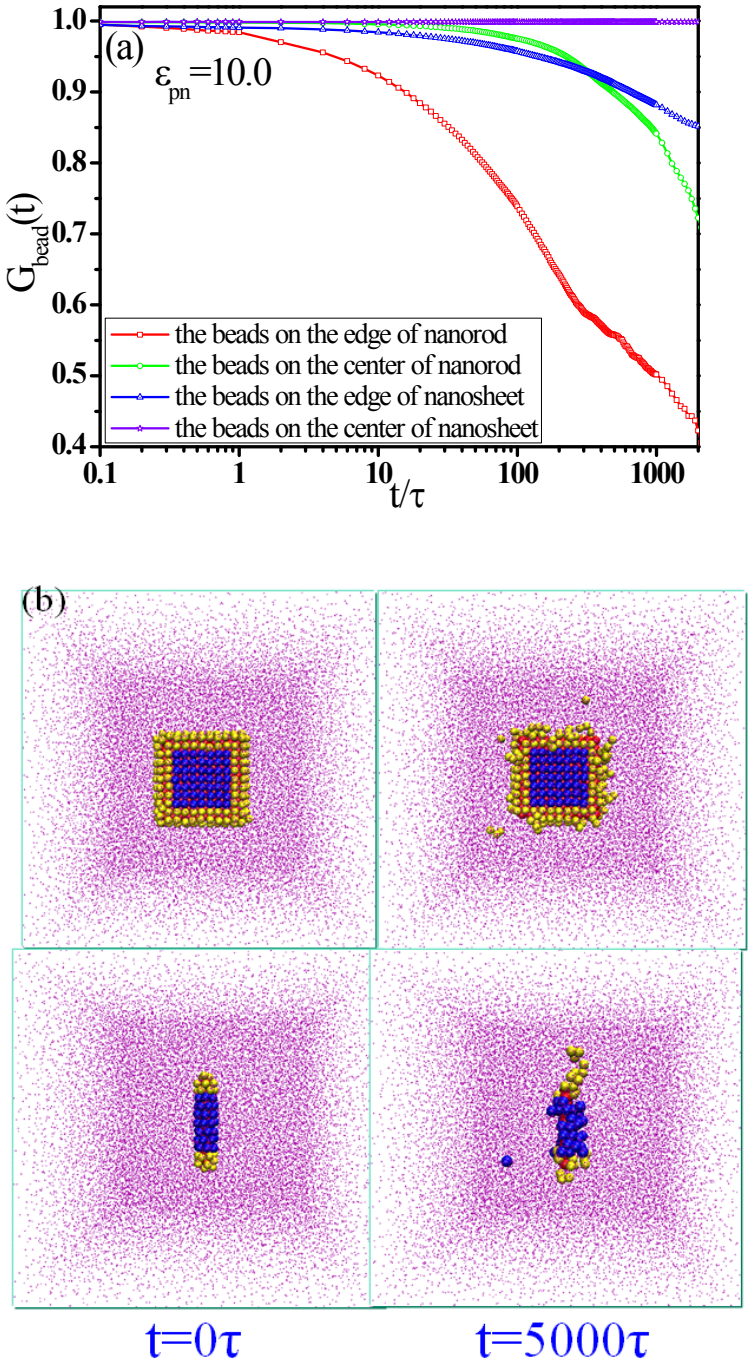


Fig. S16. (a) Decay of $G_{bead}(t)$ for polymer beads on the edge and center of nanorod and nanosheet in the L1 region at the case. (b) The snapshots for the nanosheet or nanorod filled systems at time $t = 0\tau$ and $t = 5000\tau$. The red spheres denote the nanorod or nansosheet, the yellow bead and the blue beads denote interfacial polymer beads. The purple points denote other polymer. Note $\varepsilon_{pn} = 10.0$ here.

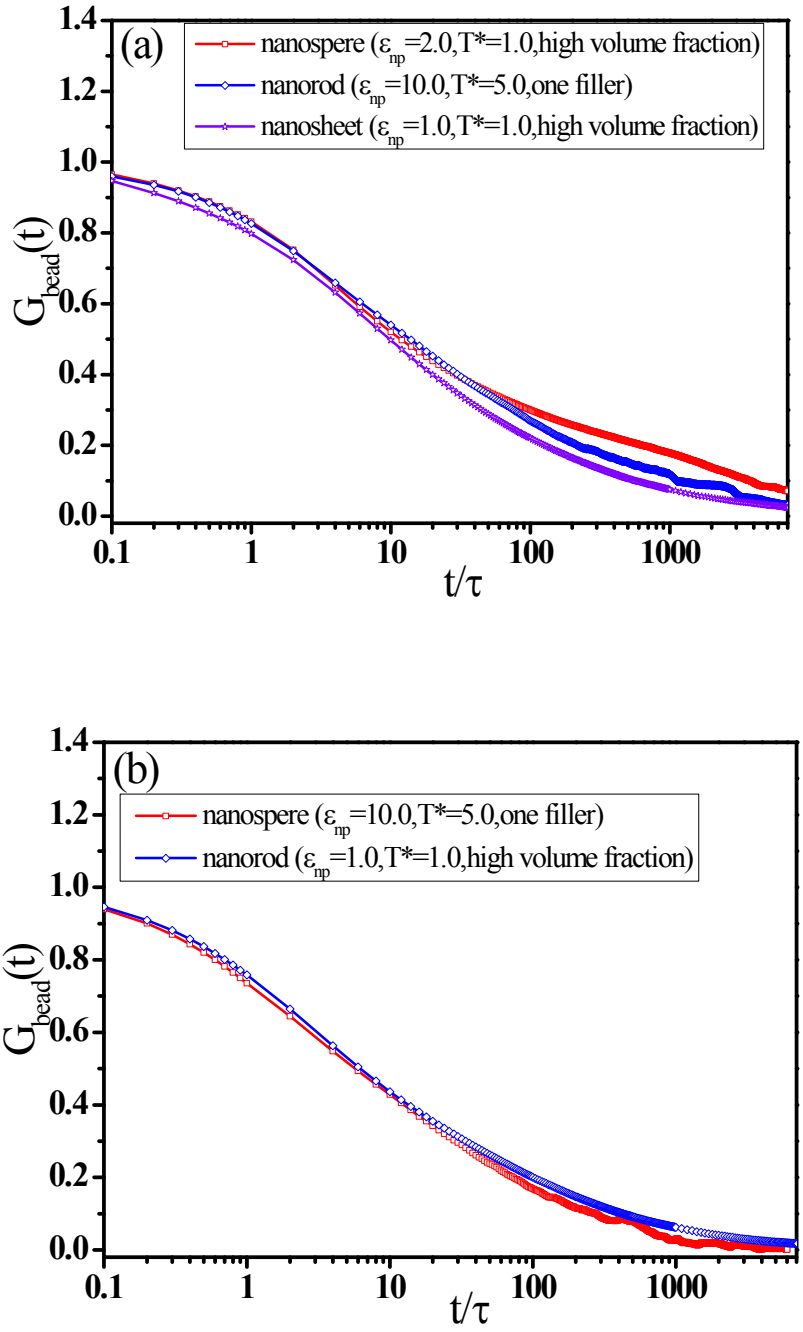


Fig. S17. Decay of $G_{bead}(t)$ for (a) three different systems, (b) two different systems.

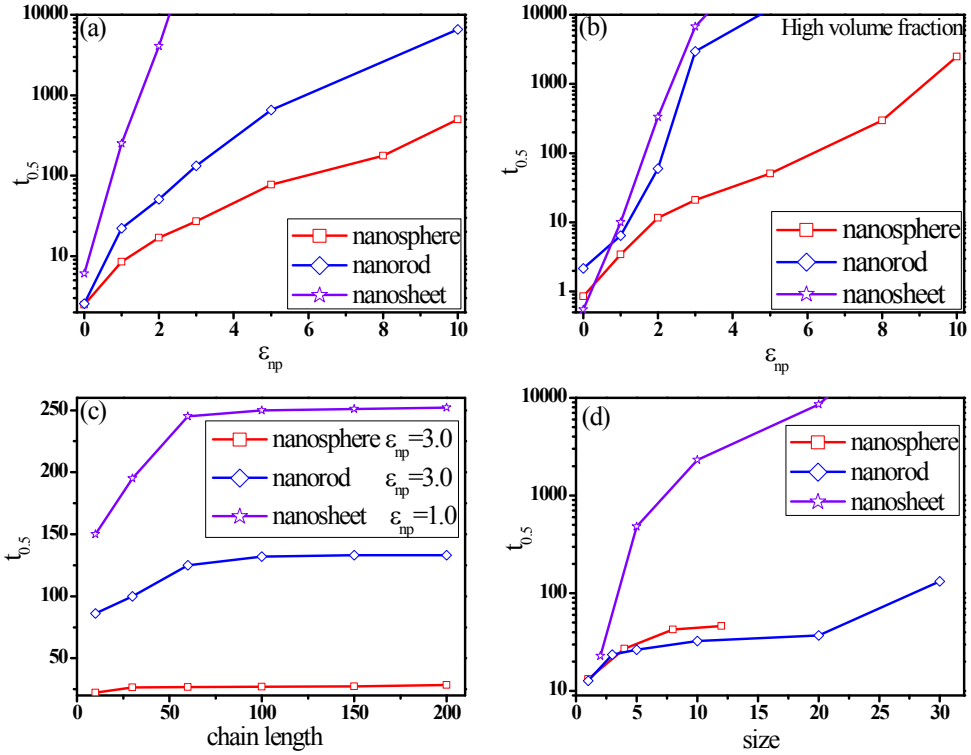


Fig. S18. The effect of (a) the interfacial interaction, (b) volume fraction of filler, (c) chain length and (d) the size of filler on the adsorption/desorption characteristic time $t_{0.5}$.