Electronic Supplementary Material (ESI) for Soft Matter.
This journal is © The Royal Society of Chemistry 2023

# Electronic Supplementary Information: Structure and dynamics of an active polymer chain inside a nanochannel grafted with polymers

Rajiblochan Sahoo[a], and Rajarshi Chakrabarti[a,*]

[a] *Department of Chemistry,*

*Indian Institute of Technology Bombay, Mumbai 400076, India*

*E-mail: rajarshi@chem.iitb.ac.in*

## I. STRUCTURAL PROPERTIES OF A POLYMER INSIDE A NANOCHANNEL WITHOUT GRAFTED POLYMERS

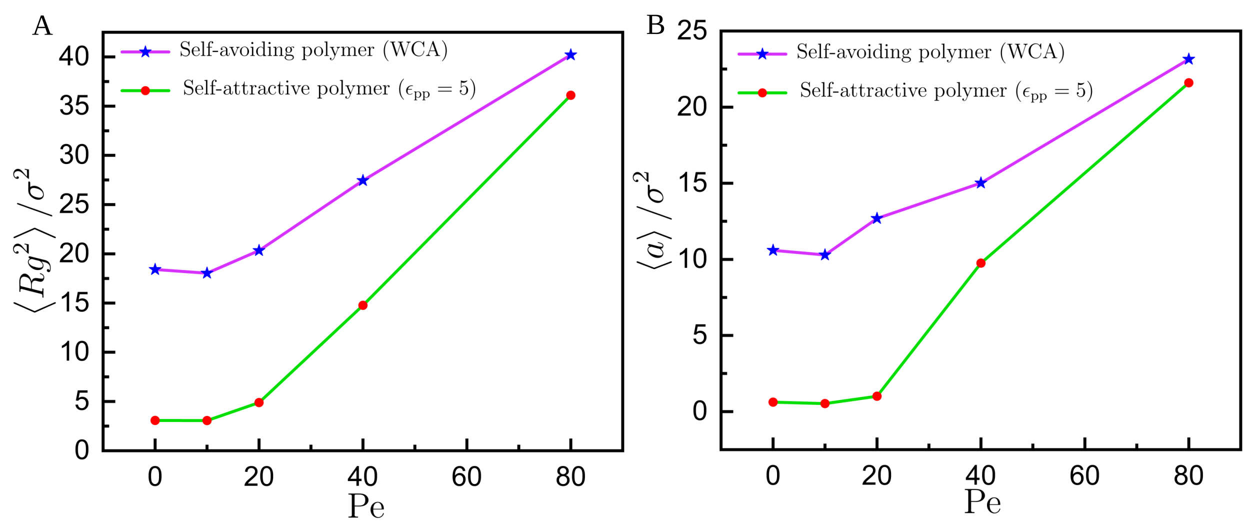


Fig. S1. (A) Plots of $\langle R_g^2 \rangle$ of self-avoiding and self-attractive probe-polymer at different Pe and (B) asphericity ($\langle a \rangle$) of self-avoiding and self-attractive probe-polymer at different Pe inside a nanochannel.

## II. STRUCTURAL PROPERTIES OF PROBE-POLYMER INSIDE NANOCHANNEL GRAFTED WITH POLYMERS

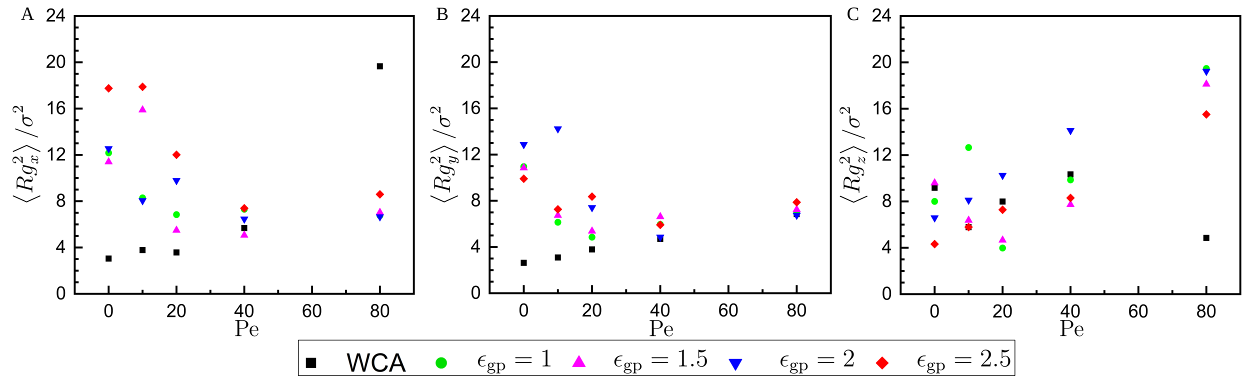


Fig. S2. (A) Plots of $\langle R_{g_x}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$, (B) Plots of $\langle R_{g_y}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$, and (C) Plots of $\langle R_{g_z}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$ for self-avoiding probe-polymer in the crowded nanochannel. Here, $\langle R_{g_x}^2 \rangle$, $\langle R_{g_y}^2 \rangle$, and $\langle R_{g_z}^2 \rangle$ are the values along x-direction, y-direction, and z-direction respectively.

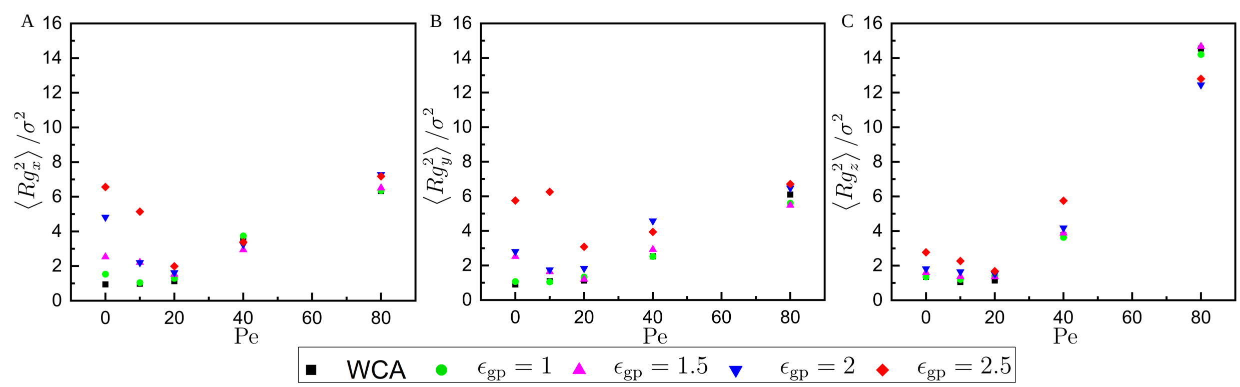


Fig. S3. (A) Plots of $\langle R_{g_x}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$, (B) Plots of $\langle R_{g_y}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$, and (C) Plots of $\langle R_{g_z}^2 \rangle$ vs. Pe as a function of $\epsilon_{\text{gp}}$ for self-attractive probe-polymer in the crowded nanochannel. Here, $\langle R_{g_x}^2 \rangle$, $\langle R_{g_y}^2 \rangle$, and $\langle R_{g_z}^2 \rangle$ are the values along x-direction, y-direction, and z-direction respectively.

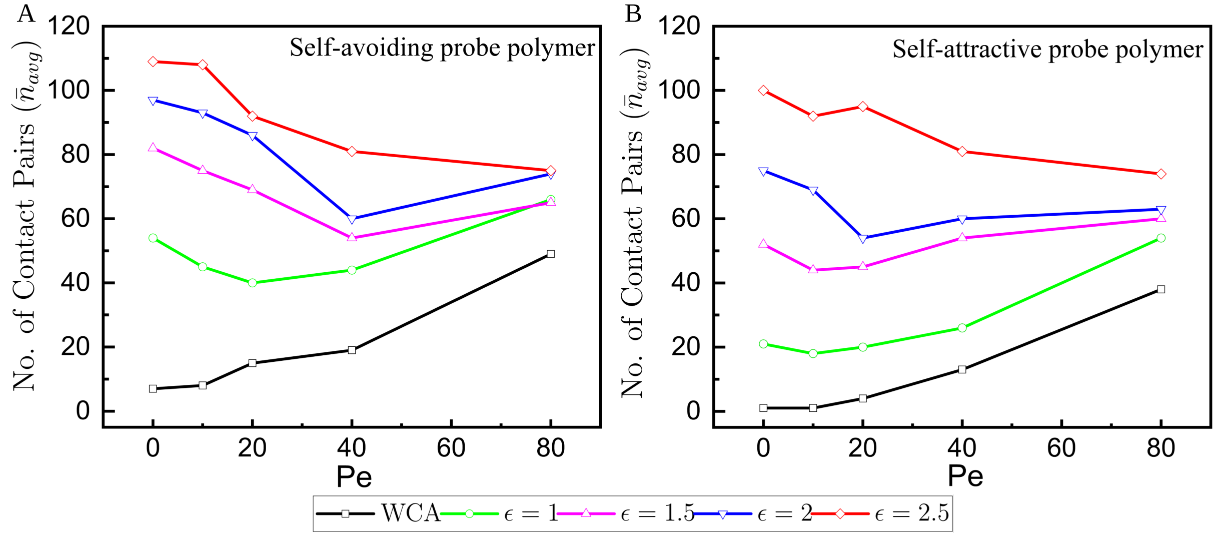


Fig. S4. (A) Contact pair between the self-avoiding probe-polymer and grafted polymers vs. Pe as a function of $\epsilon_{\rm gp}$ in the crowded nanochannel. (B) Contact pair between the self-attractive probe-polymer and grafted polymers vs. Pe as a function of $\epsilon_{\rm gp}$ in the crowded nanochannel. Here, the contact pair is calculated by taking a cutoff distance $1.12\sigma$ which is the $r_{max}$ value of WCA potential.

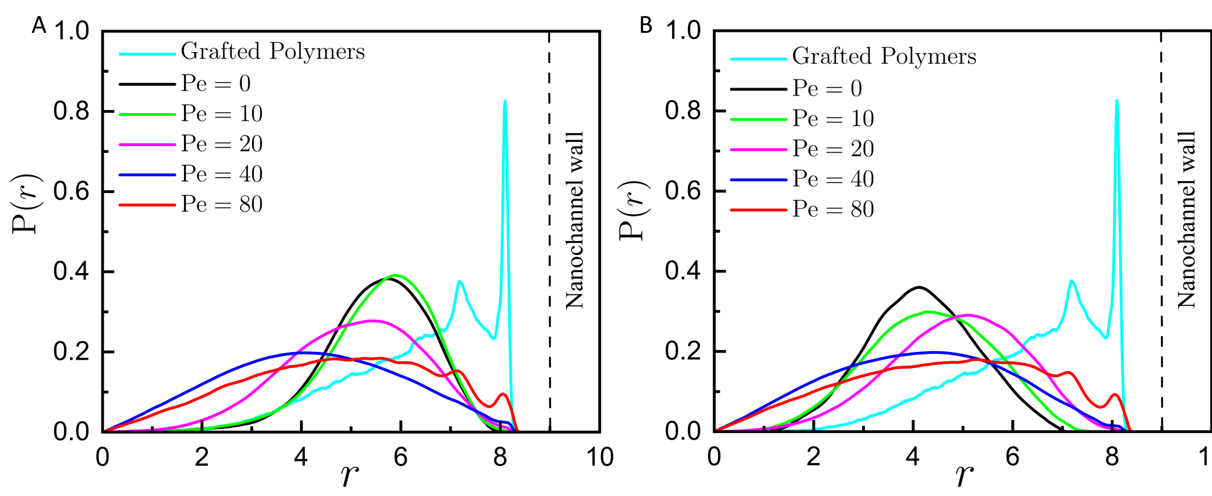


Fig. S5. Probability of finding the (A) self-avoiding probe-polymer and (B) self-attractive probe-polymer along radial direction at different Pe when the interaction is attractive ($\epsilon_{\rm gp} = 2$) with the grafted polymers.

# III. DYNAMICAL PROPERTIES OF A POLYMER INSIDE A NANOCHANNEL WITHOUT GRAFTED POLYMERS

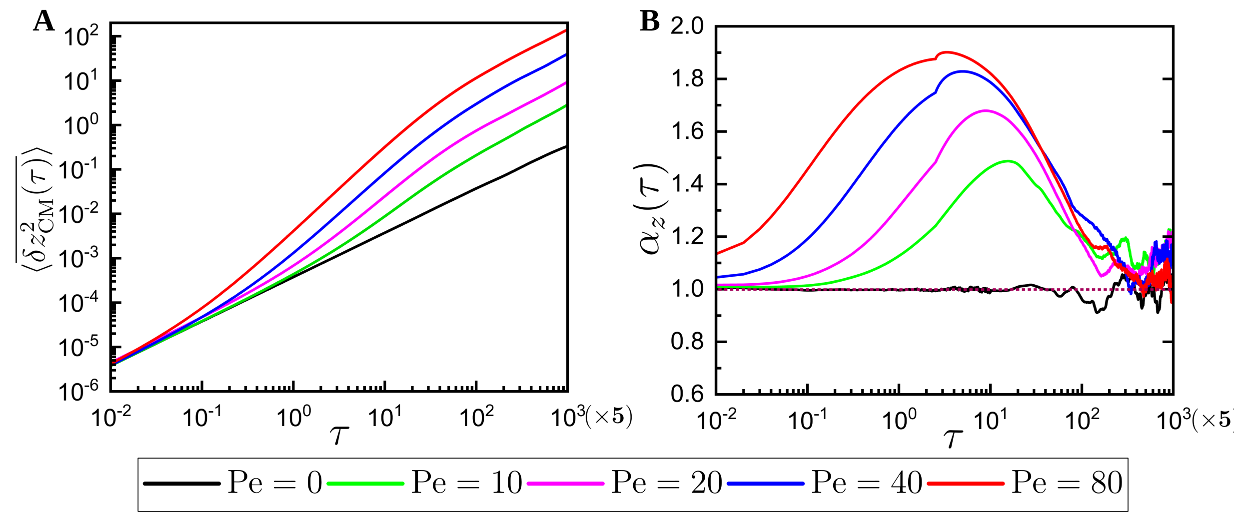


Fig. S6. (A) Log–log plot of $\left\langle \overline{\delta z^2_{\mathrm{CM}}(\tau)} \right\rangle$ vs $\tau$ and (B) log-linear plot of time-exponent of self-avoiding probe-polymer at different Pe inside a nanochannel.

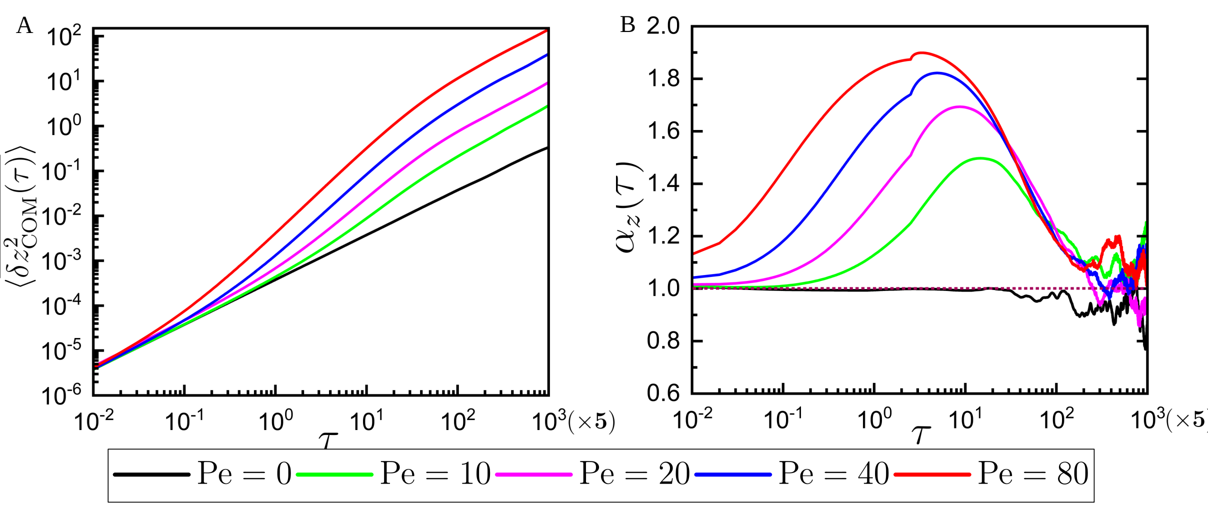


Fig. S7. (A) Log–log plot of $\left\langle \overline{\delta z^2_{\mathrm{CM}}(\tau)} \right\rangle$ vs $\tau$ and (B) log-linear plot of time-exponent of self-attractive probe-polymer at different Pe inside a nanochannel.

## IV. DYNAMICAL PROPERTIES OF PROBE-POLYMER INSIDE A NANOCHANNEL GRAFTED WITH POLYMERS

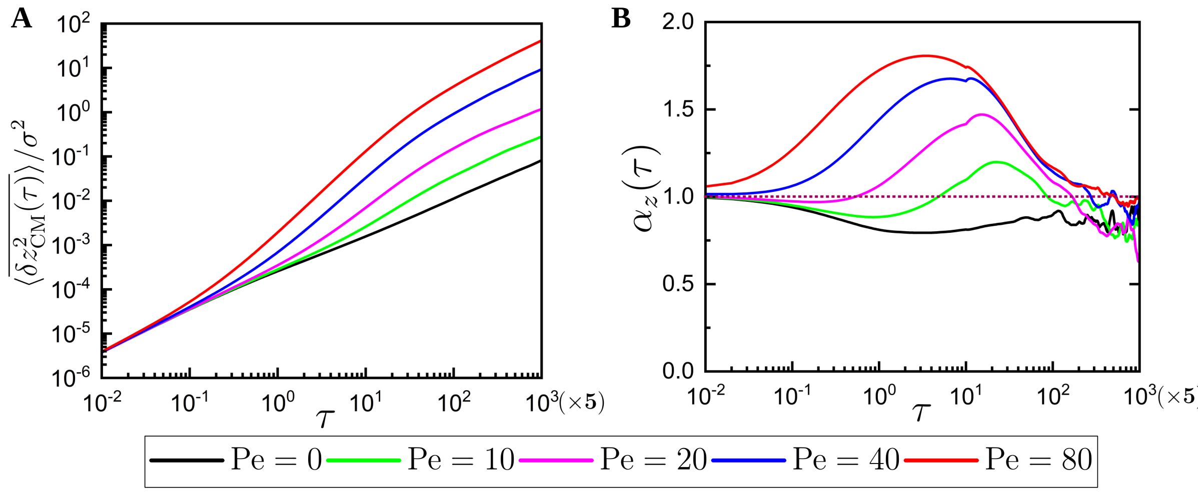


Fig. S8. (A) Log–log plot of $\left\langle\overline{\delta z^2_{\mathrm{CM}}(\tau)}\right\rangle$ vs $\tau$ and (B) log-linear plot of time-exponent when the interaction is attractive ($\epsilon_{\mathrm{gp}} = 2$) with the crowders for a self-avoiding probe-polymer at different Pe in the crowded nanochannel.

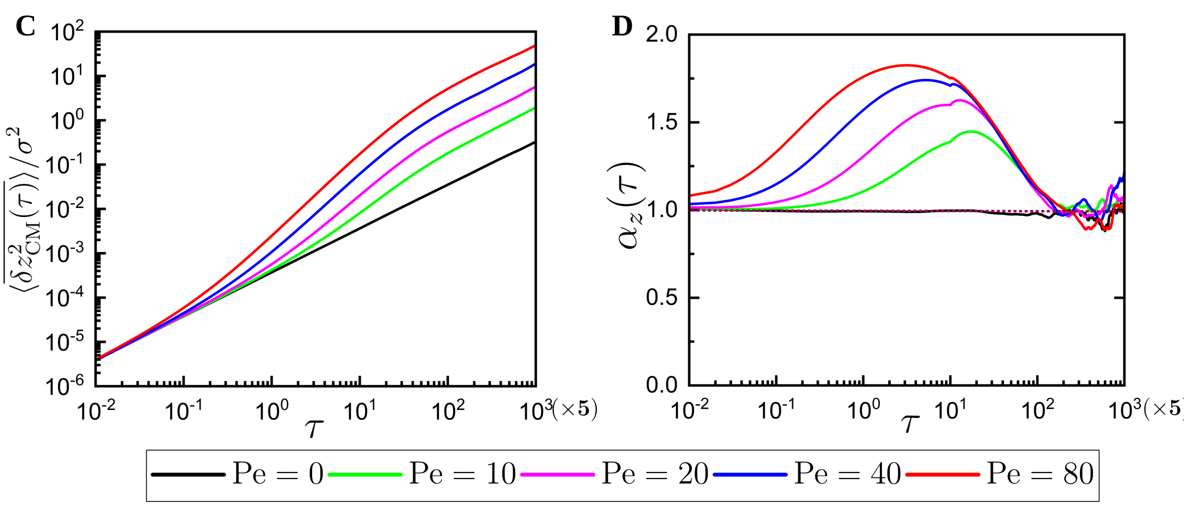


Fig. S9. (A) log–log plot of $\left\langle\overline{\delta z^2_{\mathrm{CM}}(\tau)}\right\rangle$ vs $\tau$ and (B) log-linear plot of time-exponent when the interaction is repulsive (WCA) with the crowders for a self-avoiding probe-polymer at different Pe in the crowded nanochannel.

**Movies**

The movies illustrate the qualitative difference in the dynamics of the passive and active probe-polymer inside the polymer-grafted nanochannel.

1. Movie1: Molecular dynamics simulation of the passive self-avoiding probe-polymer inside the polymer-grafted cylindrical channel with attractive interaction strength $\epsilon_{\mathrm{gp}} = 2$. The self-avoiding probe-polymer gets trapped inside the grafted polymers (top view).

2. Movie2: Side view of Movie1. Here we can see that the passive self-avoiding probe-polymer strongly interacts with the grafted polymers and tends to remain inside the grafted polymeric region.

3. Movie3: Molecular dynamics simulation of the active self-avoiding probe-polymer inside the polymer-grafted cylindrical channel with attractive interaction strength ($\epsilon_{\mathrm{gp}} = 2$) with the grafted polymers. The self-avoiding probe-polymer escape from the local trap and moves inside the polymer-grafted nanochannel (side view).

4. Movie4: Molecular dynamics simulation of the passive self-attractive probe-polymer inside the polymer-grafted cylindrical channel with attractive interaction strength $\epsilon_{\mathrm{gp}} = 2$. The self-attractive probe-polymer gets trapped inside the grafted polymers and diffusion slows down (side view).

5. Movie5: Molecular dynamics simulation of the active self-attractive probe-polymer inside the polymer-grafted cylindrical channel with attractive interaction strength ($\epsilon_{\mathrm{gp}} = 2$). Here we can see that the activity facilitates the self-attractive probe-polymer to escape from the local trap inside the grafted polymers and moves all over the area inside the channel (side view).

6. Movie6: Molecular dynamics simulation of the passive self-avoiding probe-polymer inside the polymer-grafted cylindrical channel with repulsive interaction (WCA). The self-avoiding probe-polymer diffuses through the hollow space along the cylinder axis created by the grafted polymer (top view).

7. Movie7: Side view of Movie6. It is clearly seen that the grafted polymers push the passive self-avoiding probe-polymer toward the pore-like space along the cylindrical

channel where it diffuses by adopting a compact structure.

8. Movie8: Molecular dynamics simulation of the active self-avoiding probe-polymer inside the polymer-grafted cylindrical channel with repulsive interaction strength (WCA). The self-avoiding probe-polymer escape from the grafted polymers and moves all over the area inside the polymer-grafted nanochannel (side view).

9. Movie9: Molecular dynamics simulation of the passive self-attractive probe-polymer inside the polymer-grafted cylindrical channel with repulsive interaction strength (WCA). The self-attractive probe-polymer diffuses through the hollow space along the cylinder axis created by the grafted polymer (side view).

10. Movie10: Molecular dynamics simulation of the active self-attractive probe-polymer inside the polymer-grafted cylindrical channel with repulsive interaction strength (WCA). Here we can see that the activity facilitates the self-attractive probe-polymer to escape from the local trap and moves all over the area inside the channel (side view).