Electronic Supplementary Information: Transport of a self-propelled tracer through a hairy cylindrical channel: interplay of stickiness and activity

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

[a] *Department of Chemistry,*

Indian Institute of Technology Bombay, Mumbai 400076, India

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

Figures

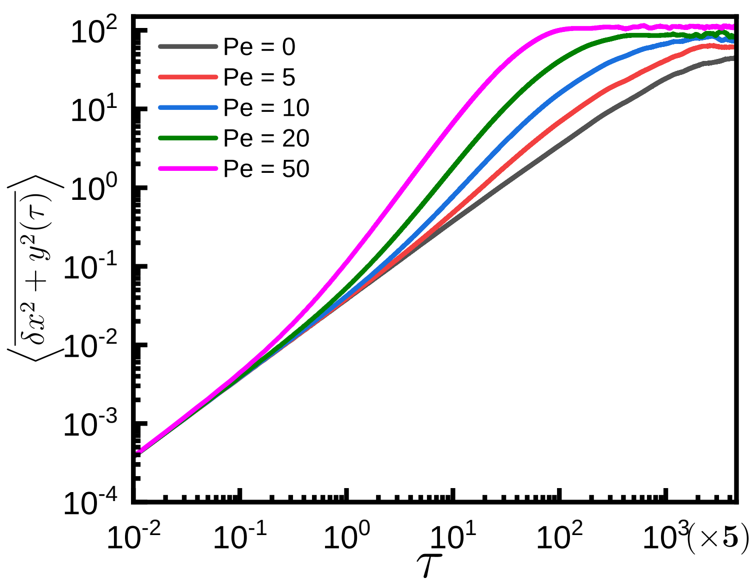


Fig. S1. Log–log plot of $\left\langle \overline{\delta(x^2 + y^2)(\tau)} \right\rangle$ vs τ of the tracer particle in cylindrical channel without polymers, at different Pe.

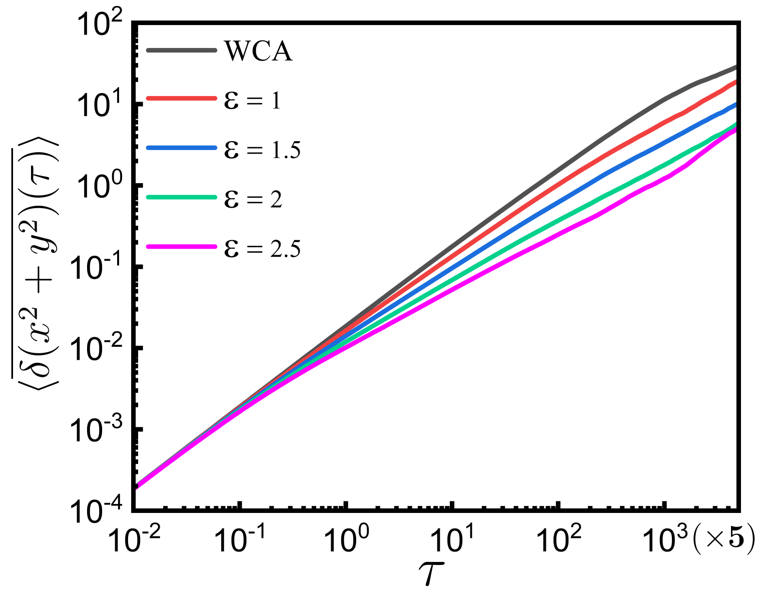
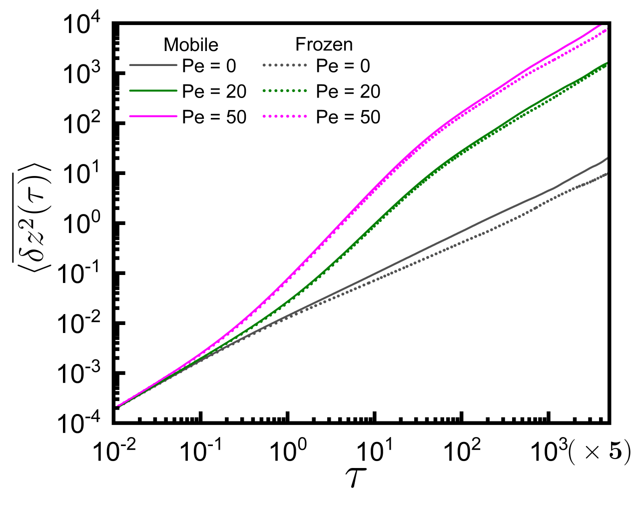
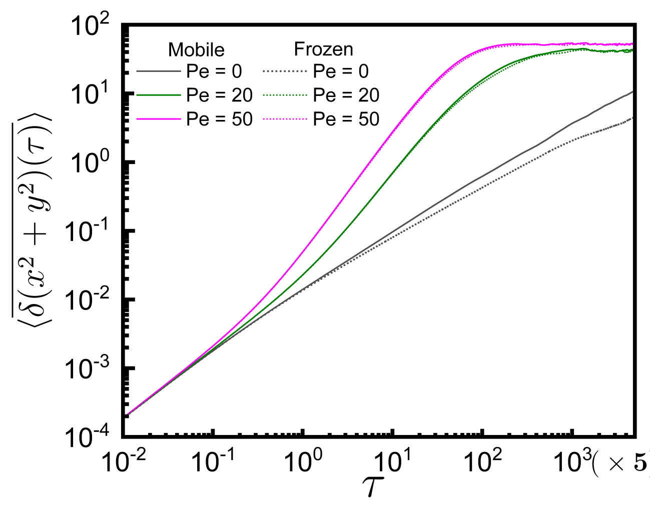


Fig. S2. Log–log plot of $\left\langle\overline{\delta(x^2+y^2)(\tau)}\right\rangle$ vs τ of the passive tracer particle in the polymer grafted cylindrical channel with different ϵ.



(a)



(b)

Fig. S3. Log–log plot of (a) $<\delta z^2(\tau)>$ vs τ and (b) $\left\langle\overline{\delta(x^2+y^2)(\tau)}\right\rangle$ vs τ for the tracer particle in the frozen polymer (dotted lines) grafted cylindrical channel and in the mobile polymer (solid lines) grafted cylindrical channel at different Pe for $\epsilon = 1.5$.

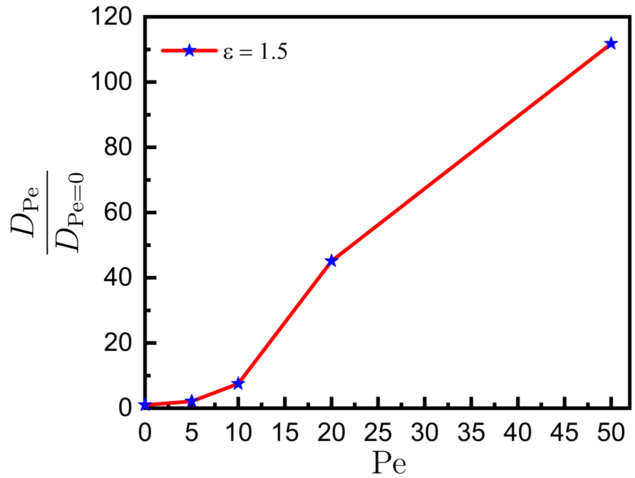


Fig. S4. $\frac{D_{\text{Pe}}}{D_{\text{Pe}=0}}$ of the tracer particle in the polymer grafted cylindrical channel at different Pe for $\epsilon = 1.5$.

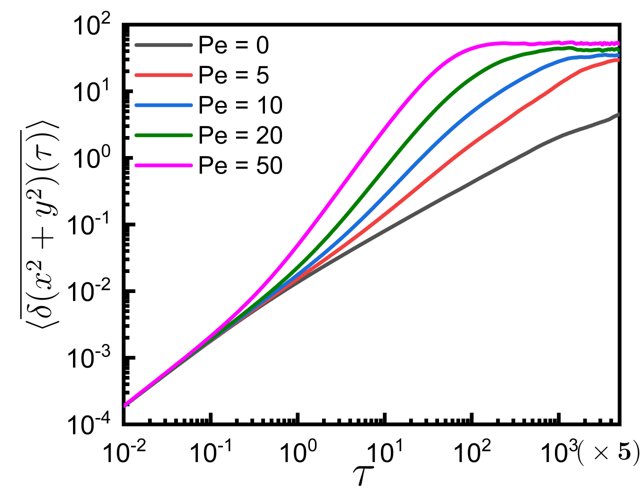
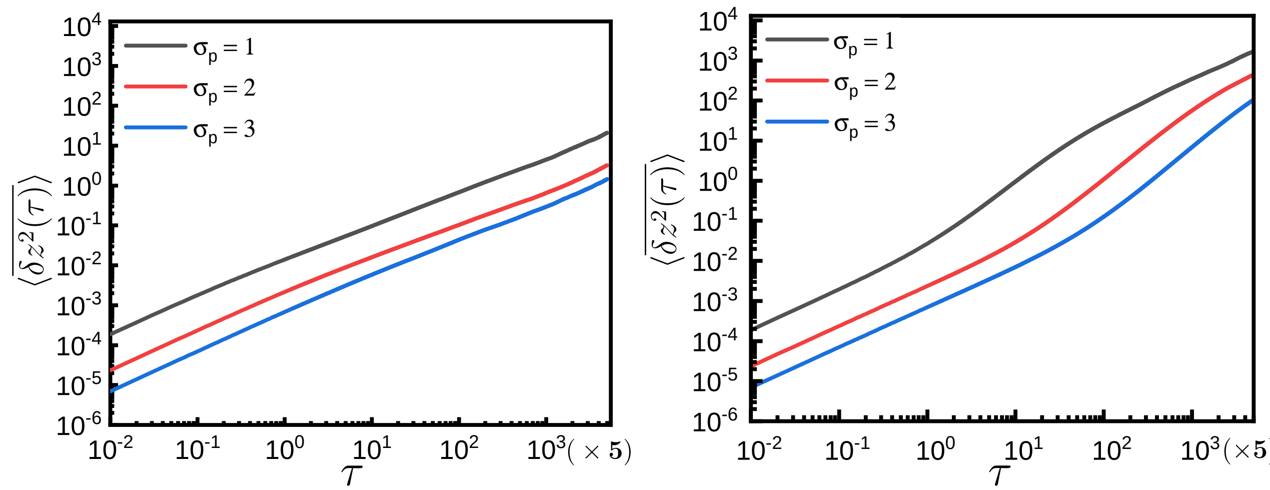
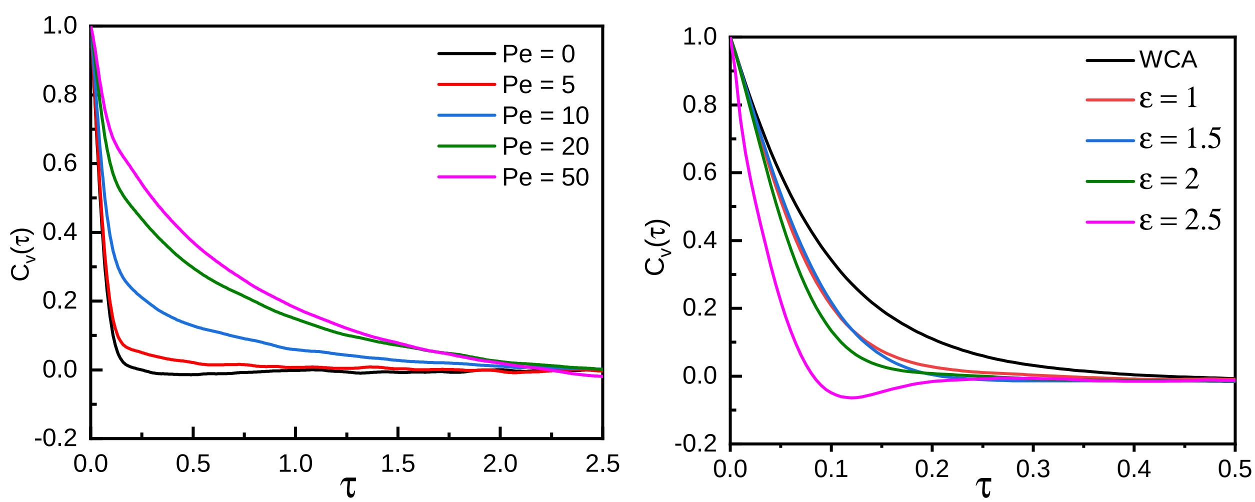


Fig. S5. Log–log plot of $\left\langle \overline{\delta(x^2+y^2)(\tau)} \right\rangle$ vs τ of the tracer particle in the polymer grafted cylindrical channel at different Pe for $\epsilon = 1.5$.



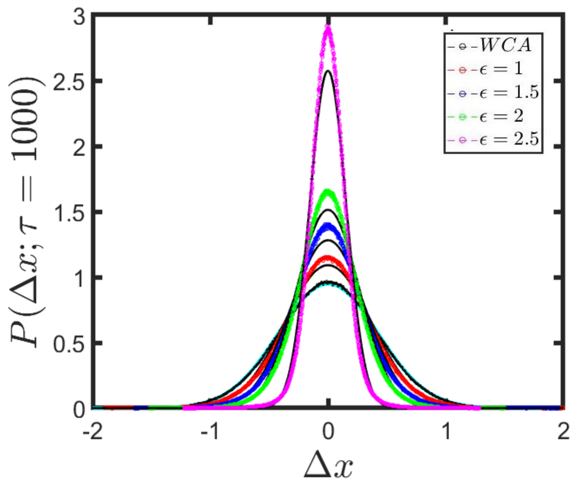
(a) (b)

Fig. S6. Log–log plot of $< \delta z^2(\tau) >$ vs τ of the tracer particle with different size for (a) Pe = 0 and (b) Pe = 20 with $\epsilon = 1.5$.

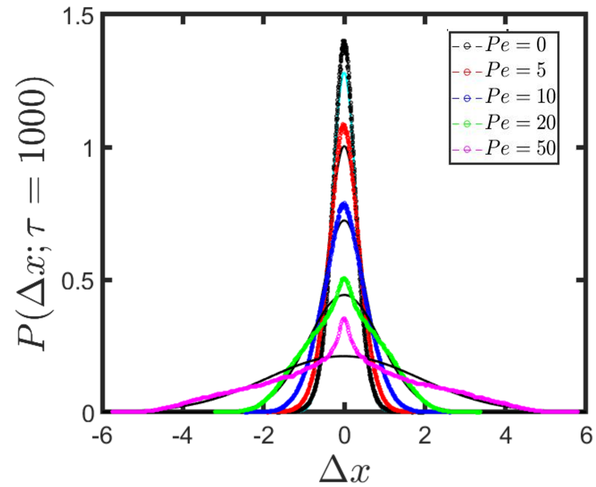


(a) (b)

Fig. S7. $C_v(\tau)$ *vs* lag time (τ) of (a) active tracer at different activity for $\epsilon = 1.5$ and (b) passive tracer with different stickiness in low friction limit.



(a)



(b)

Fig. S8. P($\Delta x; \tau$) of the tracer particle in the polymer grafted cylindrical channel with (a) different ϵ for Pe = 0 and (b) for different Pe with $\epsilon = 1.5$. The solid lines (black and cyan) represent the Gaussian fittings.

Movies

The movies illustrate the qualitative difference in the dynamics of the passive and self-propelled tracer particle in the polymer grafted cylindrical channel.

1. Movie1: Molecular dynamics simulation of the passive tracer (Pe = 0) in the polymer grafted cylindrical channel with attractive interaction strength $\epsilon = 1.5$. The tracer particle gets trapped inside the kinks in the local configuration of the grafted polymers, and then as time progresses, the polymers change their configuration, and the tracer escapes (top view).

2. Movie2: Side view of Movie1. Here we can see that the passive tracer is strongly interacting with the grafted polymers and prefer to stay in the grafted polymeric region.

3. Movie3: Molecular dynamics simulation of the self-propelled tracer (Pe = 20) in the polymer grafted cylindrical channel with attractive interaction strength $\epsilon = 1.5$. The self-propulsion force helps the tracer to escape from the local trap formed by grafted polymers, and the self-propelled tracer undergoes more random paths and explores every part of the channel (top view).

4. Movie4: Side view of Movie3. It is clearly seen that the active tracer has a tendency to move towards the grafted polymeric zone and prefers to stay close to the wall of the cylinder by following random paths.