Supplementary Information: Dynamics of a spherical self-propelled tracer in a polymeric medium: interplay of self-propulsion, stickiness and crowding

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TABLE I. Model Parameters

Parameter	**Value**
σ_{tracer}	1-4
σ_{beads}	1
$\frac{m}{\zeta}$	10^{-3}
k_BT	1
Δt	5×10^{-4}
F	0, 8, 12, 16, 20, 40
ϵ	1, 2, 3, 4, 6

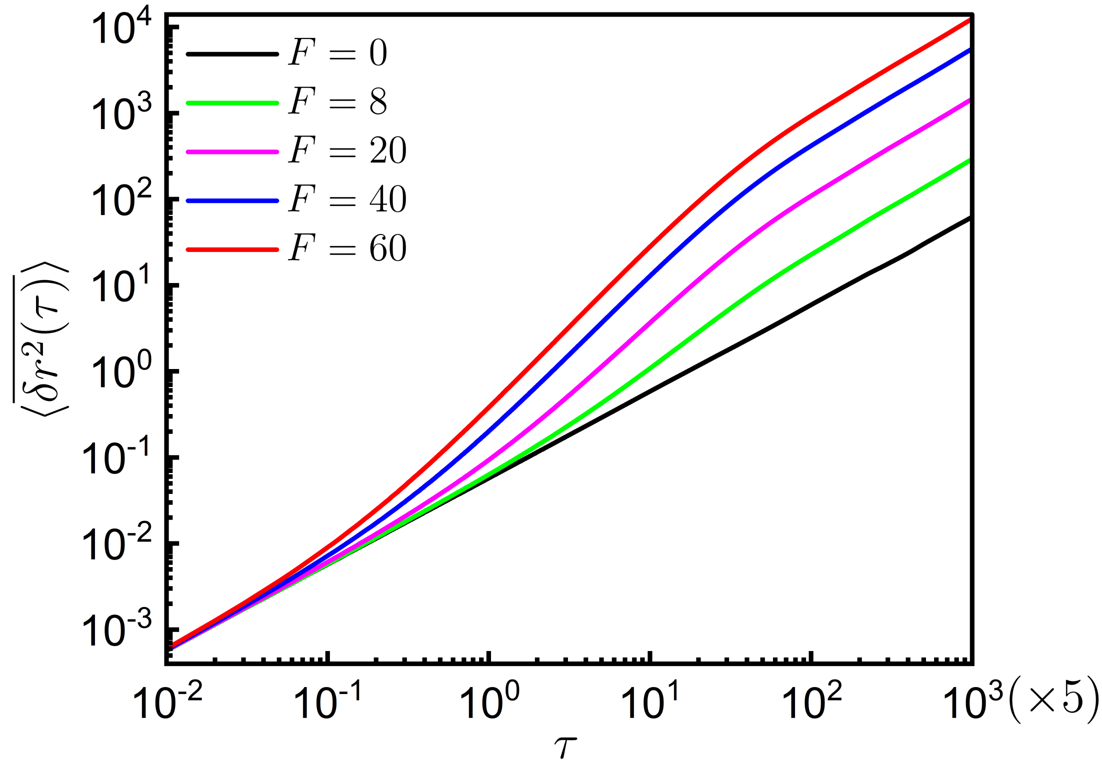

Fig. S1. Log-log plot of $\left\langle \overline{\Delta r^2(\tau)} \right\rangle$ vs τ for free particle with different F.

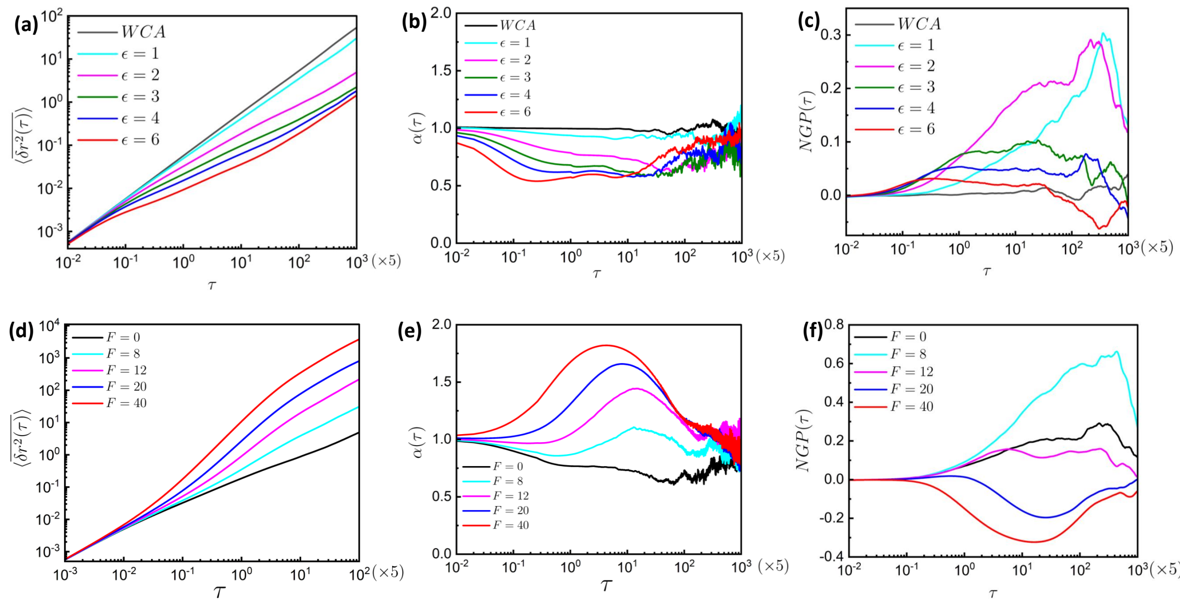

Fig. S2. Log-log plot of $\langle\overline{\delta r^2(\tau)}\rangle$ for (a) different ϵ (F = 0), (d) different F ($\epsilon = 2$), log-linear plot of $\alpha(\tau)$ for (b) different ϵ at F = 0, (e) different F at $\epsilon = 2$, NGP(τ) for(c) different ϵ at F = 0, and (f) different F for $\epsilon = 2$. (N = 200).

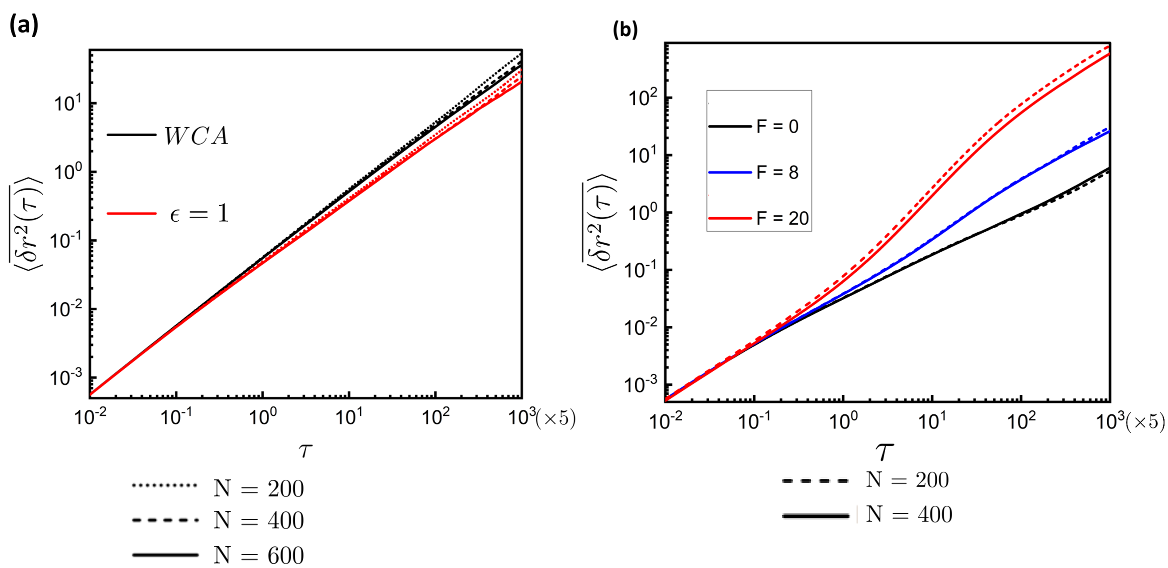

Fig. S3. Log-log plot of $\langle\overline{\delta r^2(\tau)}\rangle$ for (a) different ϵ (F = 0), (b) different F ($\epsilon = 2$).

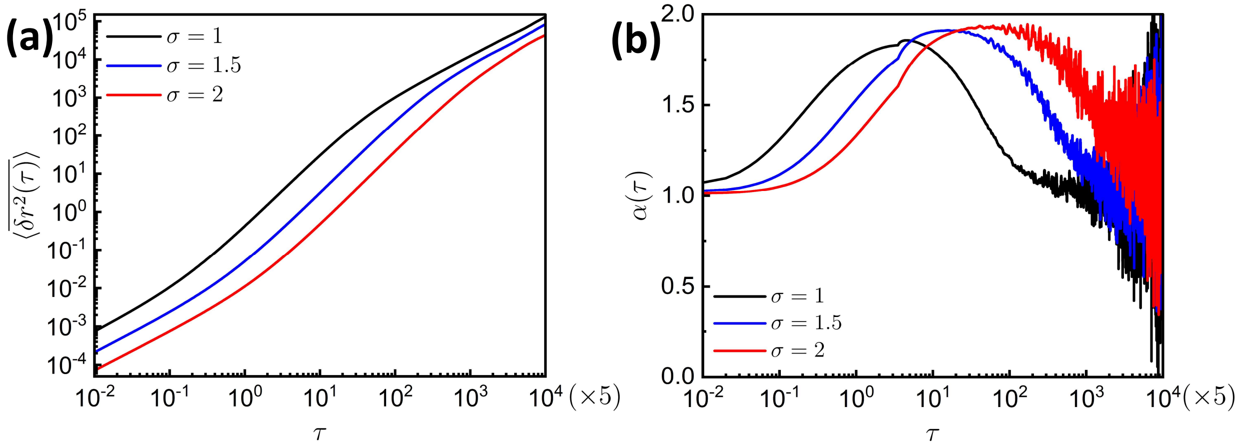

Fig. S4. (a) Log-log plot of $\left\langle \overline{\delta r^2(\tau)} \right\rangle$ and (b) log-linear plot of $\alpha(\tau)$ vs τ for different size of the tracer with constant $F = 40$, $\epsilon = 2$.

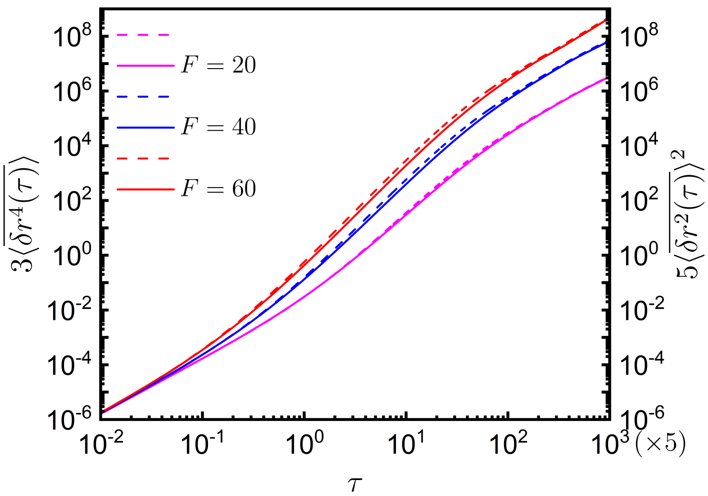

Fig. S5. Log-log plot for fourth moment of displacement $3\langle\overline{\delta r^4(\tau)}\rangle$ (solid line) and square of mean square displacement $5\langle\overline{\delta r^2(\tau)}\rangle^2$ (dotted line) vs τ for different F and $\epsilon = 2$.

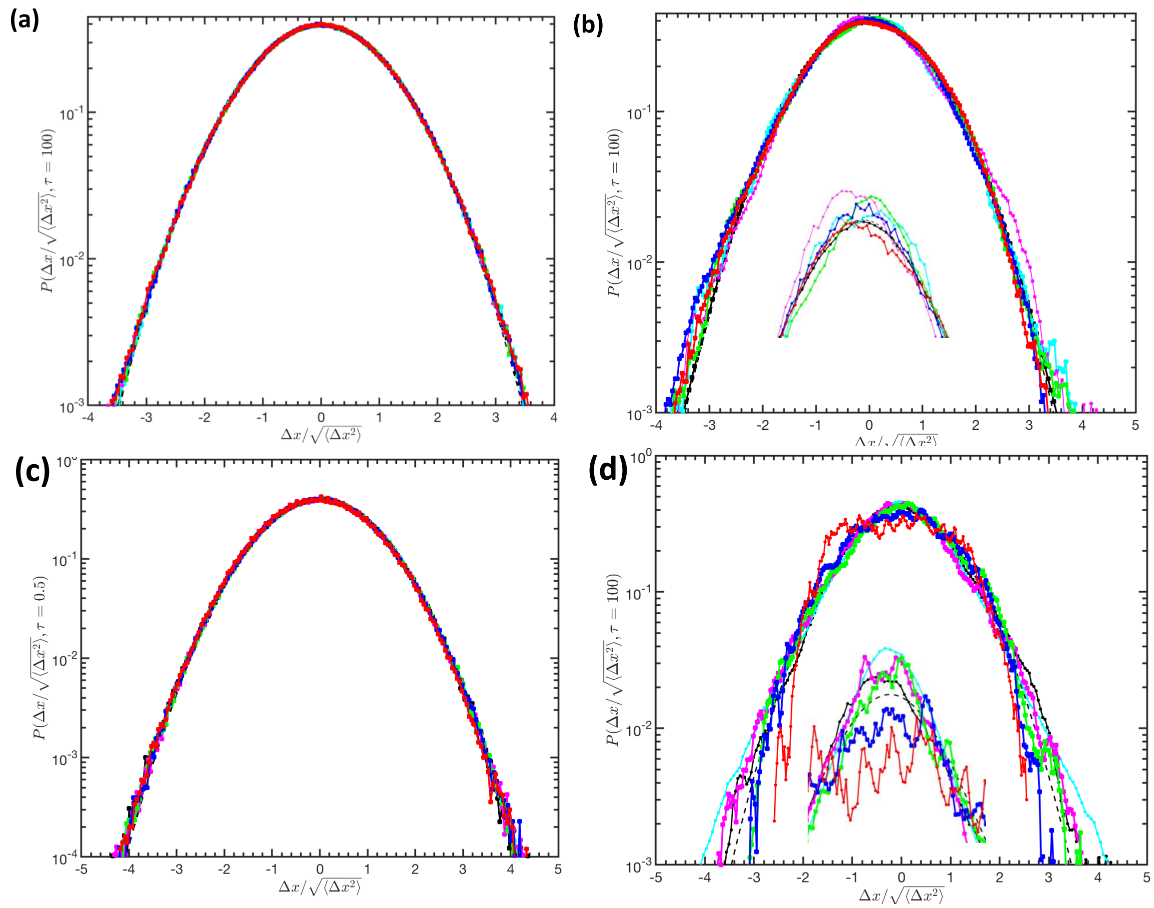

Fig. S6. Log linear plot of $P(\Delta X; \tau = 0.5)$ for (a) different ϵ at F = 0, (b) different F at $\epsilon = 2$, and $P(\Delta X; \tau = 100)$ for (c) different ϵ at F = 0, (d) different F at $\epsilon = 2$. Inset one is the enlarge peak of the distribution.

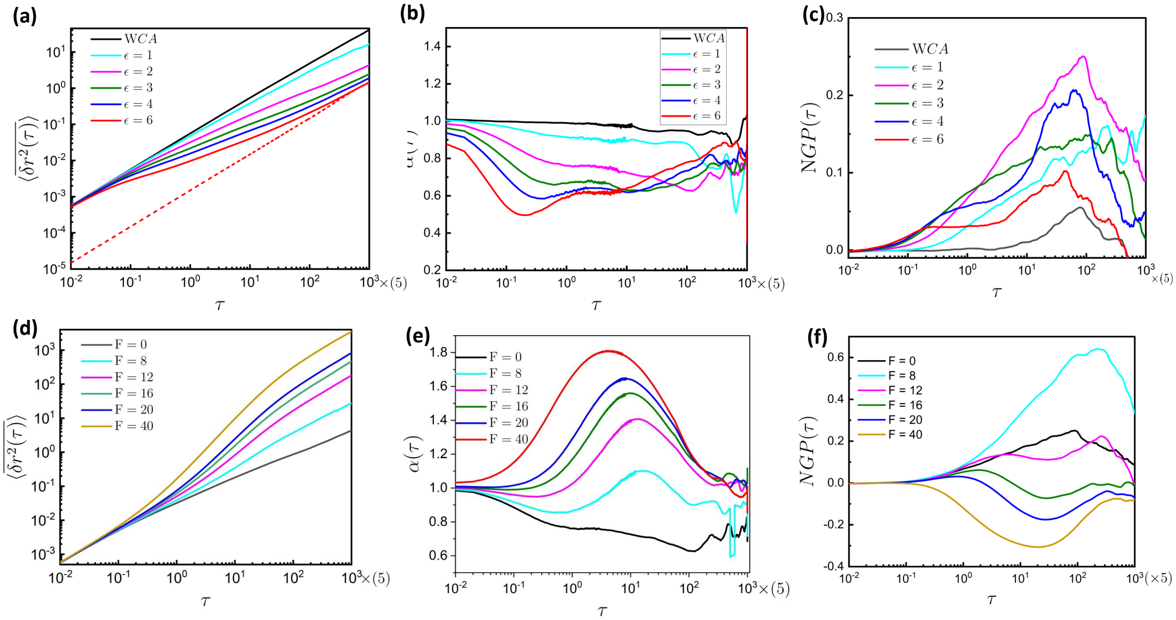

Fig. S7. Log-log plot of $\langle\overline{\delta r^2(\tau)}\rangle$ for (a) different ϵ (F = 0), (d) different F ($\epsilon = 2$)., log-linear plot of $\alpha(\tau)$ for (b) different ϵ at F = 0, (e) different F at $\epsilon = 2$, NGPτ for(c) different ϵ at F = 0, and (f) different F for $\epsilon = 2$ (N = 400, polymer with specific binding zone).

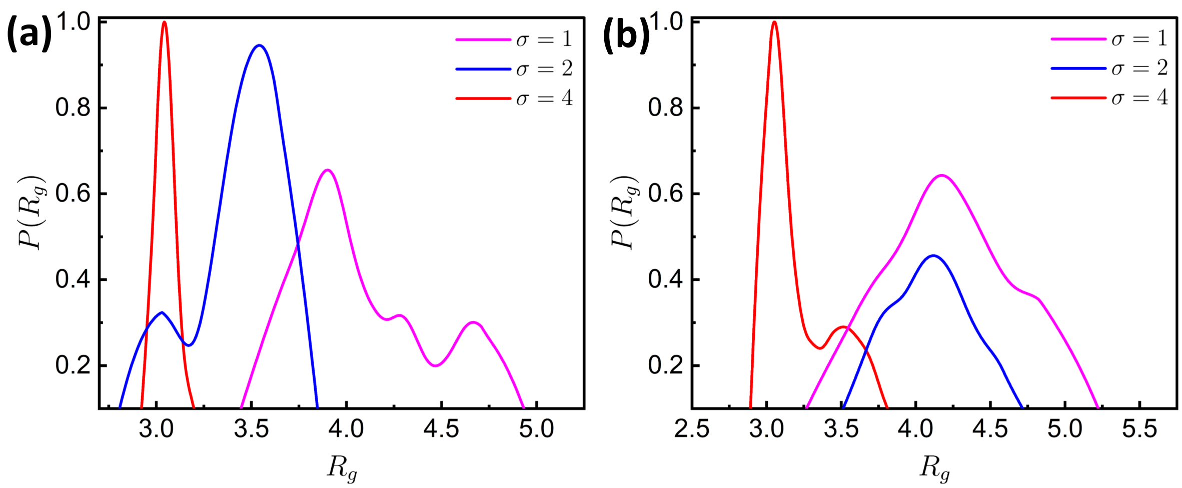

Fig. S8. Probability distribution of $R_{\rm g}$ of polymer trapping zone for (a) passive tracer particle $F = 0$, $\epsilon = 2$ and (b) self-propelled tracer particle $F = 20$, $\epsilon = 2$. (N = 200, polymer with specific binding zone.)

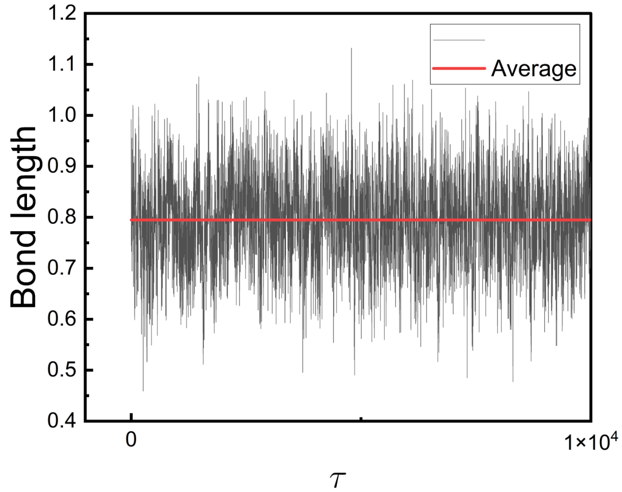

Fig. S9. plots of average bond fluctuation with time

Movie description

Movie_S1

Molecular dynamics simulation of the passive tracer particle (red) $F = 0$ in the polymeric medium consist of all sticky beads (green in color). It is clear from the movie that the passive tracer particle feel confinement by the polymer chain ($N = 400$) and the dynamics is slow.

Movie_S2

Molecular dynamics simulation of the self-propelled particle (red) $F = 8$ in the polymeric ($N = 400$) medium consist of all sticky beads (green in color). We observe that for the moderate self-propelled force propulsion enhance the dynamics of tracer particle but not necessary to overcome the stickiness and crowding effect.

Movie_S3

Molecular dynamics simulation of the self-propelled particle (red) $F = 20$ in the polymeric ($N = 400$) medium consist of all sticky beads (green in color) with all sticky beads. Here, we observe that for high self propulsion tracer particle can escape from the crowing and stickiness effect.

Movie_S4

Molecular dynamics simulation of the passive tracer particle (red) with $\sigma_{tracer} = 1$, ($F = 0$) in the polymeric ($N = 400$) medium consist of 200 sticky beads at center (green) and others are repulsive (blue). Here, the tracer particle spends maximum time in the trapping zone.

Movie_S5

Molecular dynamics simulation of the self-propelled tracer particle (red) with $\sigma_{tracer} = 1$, ($F = 8$) in the polymeric ($N = 400$) medium consist of 200 sticky beads at centre (green) and others are repulsive (blue). Here the particle escapes from the trapping zones due to self-propulsion.

Movie_S6

Molecular dynamics simulation of the self-propelled tracer particle (red) with $\sigma_{tracer} = 4$,

($F = 20$) in the polymeric ($N = 400$) medium consist of 200 sticky beads at centre (green) and others are repulsive (blue). The trapping zones of polymer is getting collapse due to strong sticky interactions of tracer particle.

Movie_S7

Molecular dynamics simulation of the passive tracer particle (red) with $\sigma_{tracer} = 4$, ($F = 0$) in the polymeric ($N = 200$) medium consist of 100 sticky beads at centre (green) and others are repulsive (blue). The trapping zones of polymer is getting collapse and fluctuate due to larger size of tracer particle and activity of the tracer particle.

Movie_S8

Molecular dynamics simulation of the self-propelled tracer particle (red) with $\sigma_{tracer} = 4$, ($F = 20$) in the polymeric ($N = 200$) medium consist of 100 sticky beads at centre (green) and others are repulsive (blue). The trapping zones of polymer shows less collapse and fluctuate due to larger size of tracer particle and activity of the tracer particle.