Electronic Supplementary Information: Dynamics of self-propelled tracer particles inside a polymer network

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To characterize the polymer network which is constructed on a diamond lattice, we measure the average mesh size of the polymer network by considering distances between the nearest monomers of the network as shown in Fig. S1.

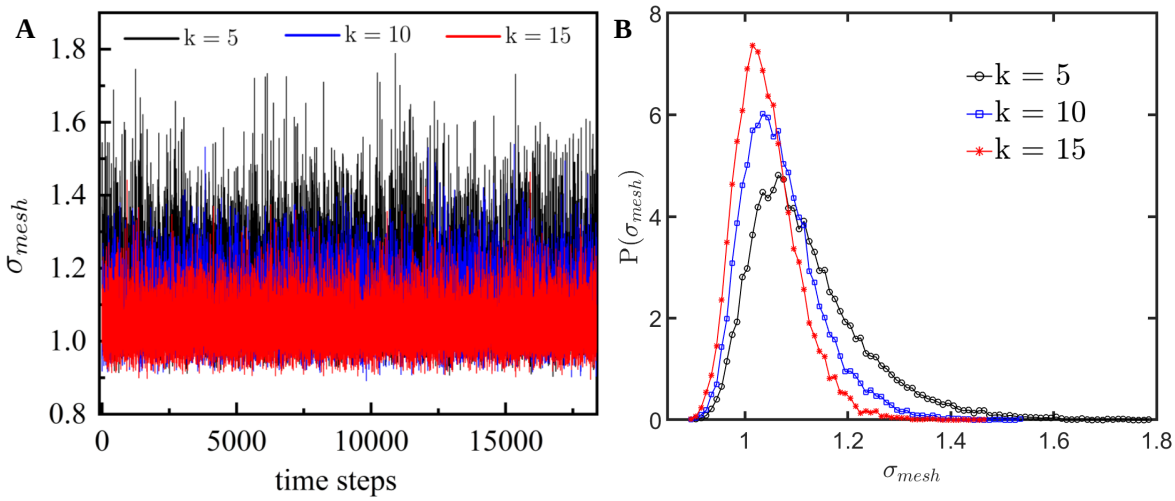

Fig. S1. Plots of (A) the mesh size fluctuation (σ_{mesh}) *vs* time steps and (B) mesh size distribution P(σ_{mesh}) of the polymer network.

For method and parameter validation, we carried out the simulations of an active Brownian particle (ABP) in free space. The time-averaged mean-squared displacement $\left(\left\langle\overline{\Delta r^2(\tau)}\right\rangle\right)$ is calculated. From the plot (Fig. S2) for $F_a = 0$, first we have computed the thermal translational diffusion coefficient, $D_t = 9.35 \times 10^{-5}$ and then rotational diffusion coefficient, $D_R = 2.8 \times 10^{-4}$ by using the expression, $D_r = \frac{3D_t}{\sigma^2}$, where σ is the size of an ABP. Thus, the persistence time is, $\tau_R = \frac{1}{2D_r} = 1.8 \times 10^3$. Using the values of D_t and τ_R, $\left\langle\overline{\Delta r^2(\tau)}\right\rangle$ is

fitted with the analytical expression for ABP:

$$\left\langle \Delta r^2(\tau) \right\rangle = 6D_t\tau + \frac{2\mathrm{F_a^2}\tau_R}{\gamma^2}\left[\tau + \tau_R\left(e^{-\frac{\tau}{\tau_R}} - 1\right)\right] \tag{1}$$

For the passive case ($\mathrm{F_a} = 0$), $\left\langle \overline{\Delta r^2(\tau)} \right\rangle$ is always diffusive $\left(\left\langle \overline{\Delta r^2(\tau)} \right\rangle \sim \tau\right)$ with the diffusion coefficient D_t. In case of self-propelled tracer, $\left\langle \overline{\Delta r^2(\tau)} \right\rangle$ exhibits three distinct regions: diffusive at short time ($\tau < \tau_R$), superdiffusive region at intermediate time ($\tau \simeq \tau_R$) which scales as $\left\langle \overline{\Delta r^2(\tau)} \right\rangle \sim \tau^2$, followed by enhanced diffusive region at longer time, *i.e.* $\tau > \tau_R$ and the expression becomes $\langle \Delta r^2(\tau) \rangle = (6D_t + \frac{2\mathrm{F_a^2}\tau_R}{\gamma^2})\tau$. $\left\langle \overline{\Delta r^2(\tau)} \right\rangle$ grows faster with $\mathrm{F_a}$ in comparison to the passive tracer (shown in Fig. S2).

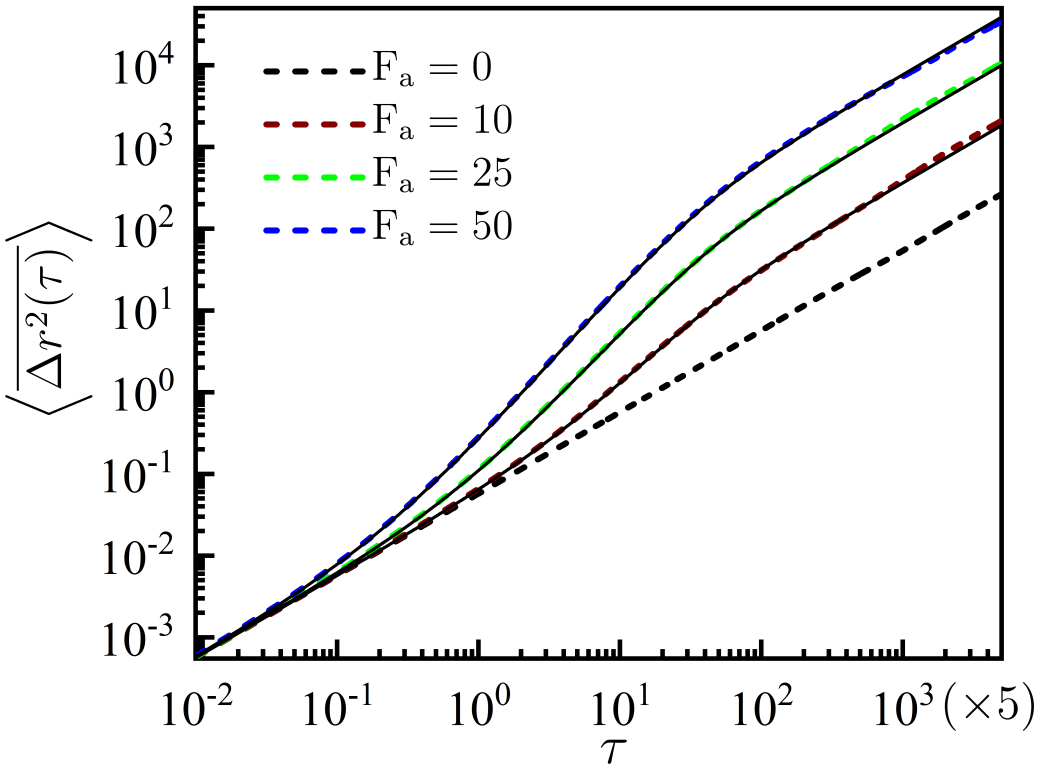

Fig. S2. Log-log plot of (A) $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ fitted with Eq. (1) (solid black lines) for the self-propelled tracer particle (ABP) in free space for various $\mathrm{F_a}$.

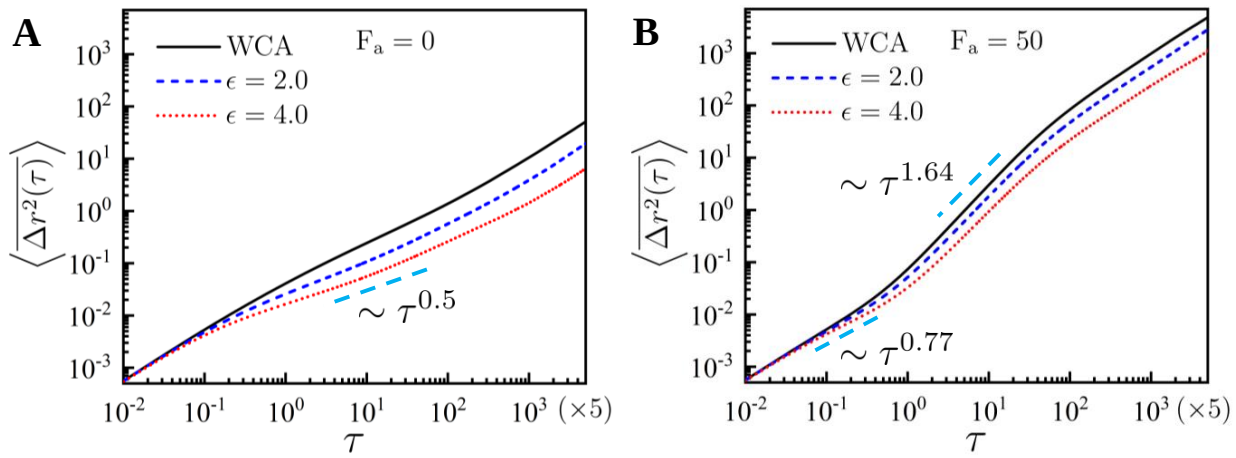

Fig. S3. Log-log plots of $\left\langle \overline{\Delta r^2(\tau)} \right\rangle$ *vs* τ of the (A) passive ($F_a = 0$) and (B) active ($F_a = 50$) tracers inside the polymer network by varying the interaction of the tracers with the monomer of the network at $\sigma = 1.0$ and $k = 10$.

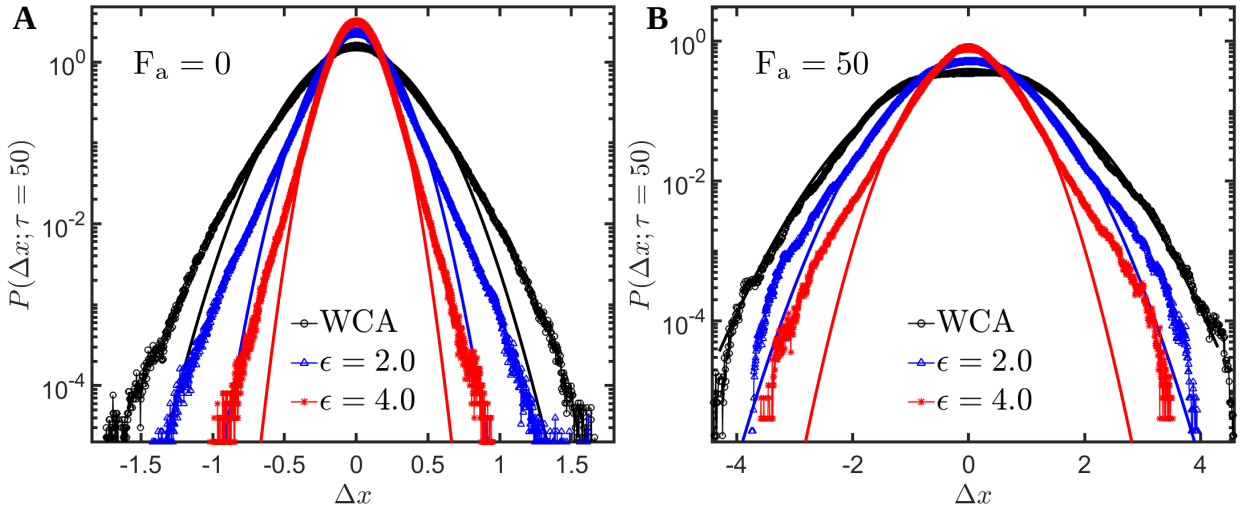

Fig. S4. $P(\Delta x; \tau)$ of the (A) passive ($F_a = 0$) and (B) active ($F_a = 50$) tracers inside the polymer network for different interaction of the tracer particles with network at $\sigma = 1.0$, $k = 10$, and lag time $\tau = 50$. Solid lines represent the best Gaussian fits.

Movie description

Movie S1

Molecular dynamics simulation of the passive ($F_a = 0$) tracer particles (red in color) and it is clear from the movie passive tracers are transiently trapped inside the polymer network.

Movie S2

Molecular dynamics simulation of the self-propelled ($F_a = 50$) tracer particles. One can see that the self-propulsion helps the tracer to escape from the polymer meshes and it covers a larger space inside the network.

Movie S3

Molecular dynamics simulation of the relatively bigger particles ($\sigma = 1.5$) for $F_a = 0$. Here, passive particles are trapped inside the meshes formed by the polymer network.

Movie S4

Molecular dynamics simulation of the relatively bigger particles ($\sigma = 1.5$) for $F_a = 50$. Here, the dynamics of self-propelled tracer particles becomes faster leading to escape dynamics from the meshes of the polymer network.