Electronic Supplementary Information: Chemically symmetric and asymmetric self-driven rigid dumbbells in 2D gel

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To characterize the polymer gel, we measure the average mesh size of the polymer gel by considering the diagonal distances between the monomers of the hexagons which is the basic repeating unit of the polymer gel as shown in Fig. S1.

The method and parameter validation is carried out for a rigid dumbbell in free space. The translational $\left(\left\langle\overline{\Delta r_c^2(\tau)}\right\rangle\right)$ and rotational $\left(\left\langle\overline{\Delta r_\theta^2(\tau)}\right\rangle\right)$ mean square displacement are calculated. From the plot (Fig. S2) for Pe = 0, we have computed the thermal translational diffusion coefficient, $D_T = 3.79 \times 10^{-4}$ and the rotational diffusion coefficient, $D_R = 2.40 \times 10^{-3}$. Thus, the persistence time $\tau_R = \frac{1}{D_R} = 4.16 \times 10^2$. The self-propulsion velocity is $v = \frac{F_a}{\gamma}$. Using the values of D_T and τ_R, $\left\langle\overline{\Delta r_c^2(\tau)}\right\rangle$ is fitted with the analytical expression for an active Brownian particle:

$$\left\langle\overline{\Delta r_c^2(\tau)}\right\rangle = \left[4D_T + v^2\tau_R\right]\tau + \frac{v^2\tau_R^2}{2}\left[e^{-\frac{2\tau}{\tau_R}} - 1\right] \tag{1}$$

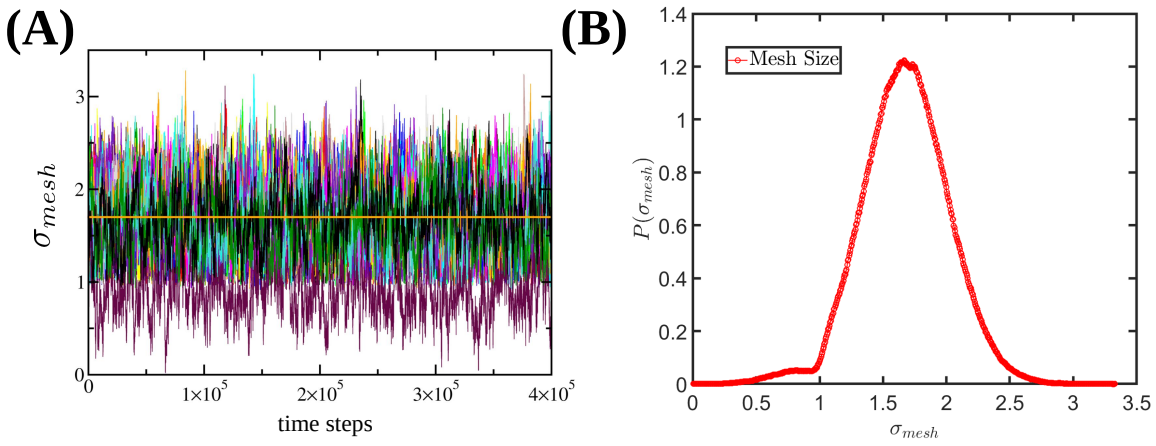

Fig. S1. Plots of (A) the mesh size fluctuation (σ_{mesh}) *vs* time steps with an average mesh size ~ 1.7 (yellow solid line) and (B) mesh size distribution P(σ_{mesh}) of the polymer gel.

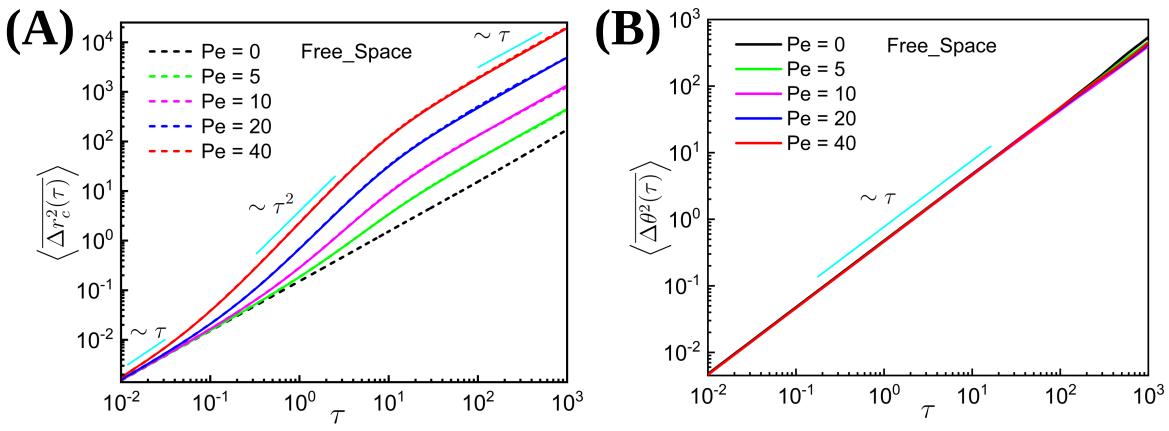

Fig. S2. log-log plot of (A) $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ fitted with Eq. (1) (solid lines) and (B) $\left\langle \overline{\Delta \theta^2(\tau)} \right\rangle$ for the self-propelled rigid dumbbell in free space at different Pe.

For the passive rigid dumbbell (Pe = 0), $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ is always diffusive $\left(\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle \sim \tau \right)$ in whole range of time with the diffusion coefficient D_T. In case of self-driven rigid dumbbell, $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ exhibits three distinct regions: diffusive at very short time ($\tau << \tau_R$) with the analytical expression $\langle \Delta r_c^2(\tau) \rangle = 4D_T\tau$, a superdiffusive region at intermediate time ($\tau \simeq \tau_R$) which scales as $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle \sim \tau^2$, and the expression becomes $\langle \Delta r_c^2(\tau) \rangle = 4D_T\tau + 2v^2\tau^2$, followed by enhanced diffusive region at longer time, *i.e.* $\tau >> \tau_R$ and the expression becomes $\langle \Delta r_c^2(\tau) \rangle = (4D_T + 2v^2\tau_R)\tau$. $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ grows faster with Pe in comparison to the passive dumbbell (shown in Fig. S2A). On the other hand, $\left\langle \overline{\Delta \theta^2(\tau)} \right\rangle$ of rigid dumbbell remains independent of self-propulsion in free space *i.e.* motion is diffusive with constant rotational diffusion coefficient $D_R = 2.40 \times 10^{-3}$, shown in Fig. S2B, which depicts that the persistence time $\tau_R = 4.16 \times 10^2$ is same for all the curves with different Pe in free space. It is due to the fact that in free space the rotation is governed only by thermal fluctuations.

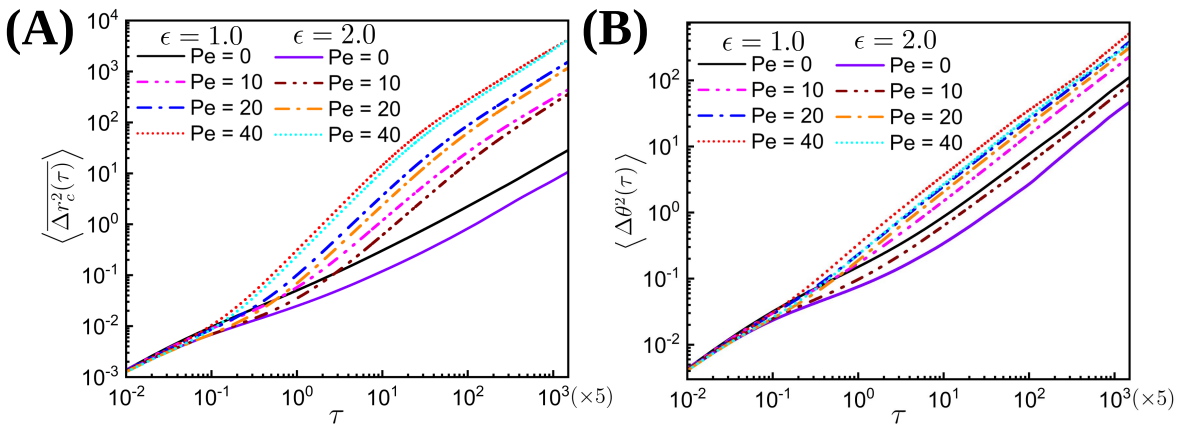

Fig. S3. log-log plots of (A) $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ *vs* τ, and (B) $\left\langle \overline{\Delta\theta^2(\tau)} \right\rangle$ *vs* τ for the attractive ($\epsilon = 1.0$ and 2.0) self-driven symmetric dumbbell in polymer gel at different Pe.

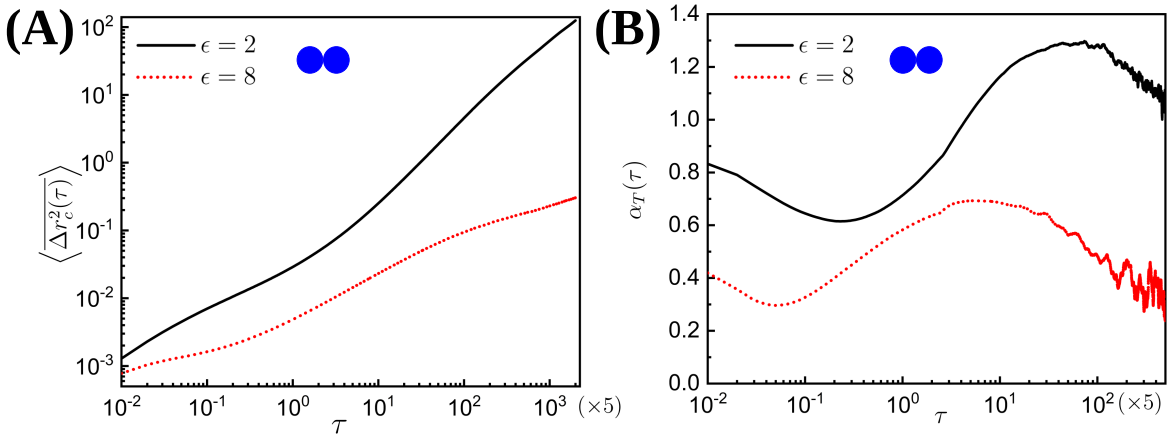

Fig. S4. log-log plot of (A) $\left\langle \overline{\Delta r_c^2(\tau)} \right\rangle$ *vs* τ and log-linear plot of (B) $\alpha_T(\tau)$ *vs* τ for the attractive ($\epsilon = 2.0$ and 8.0) self-driven symmetric dumbbell in polymer gel at Pe = 5.

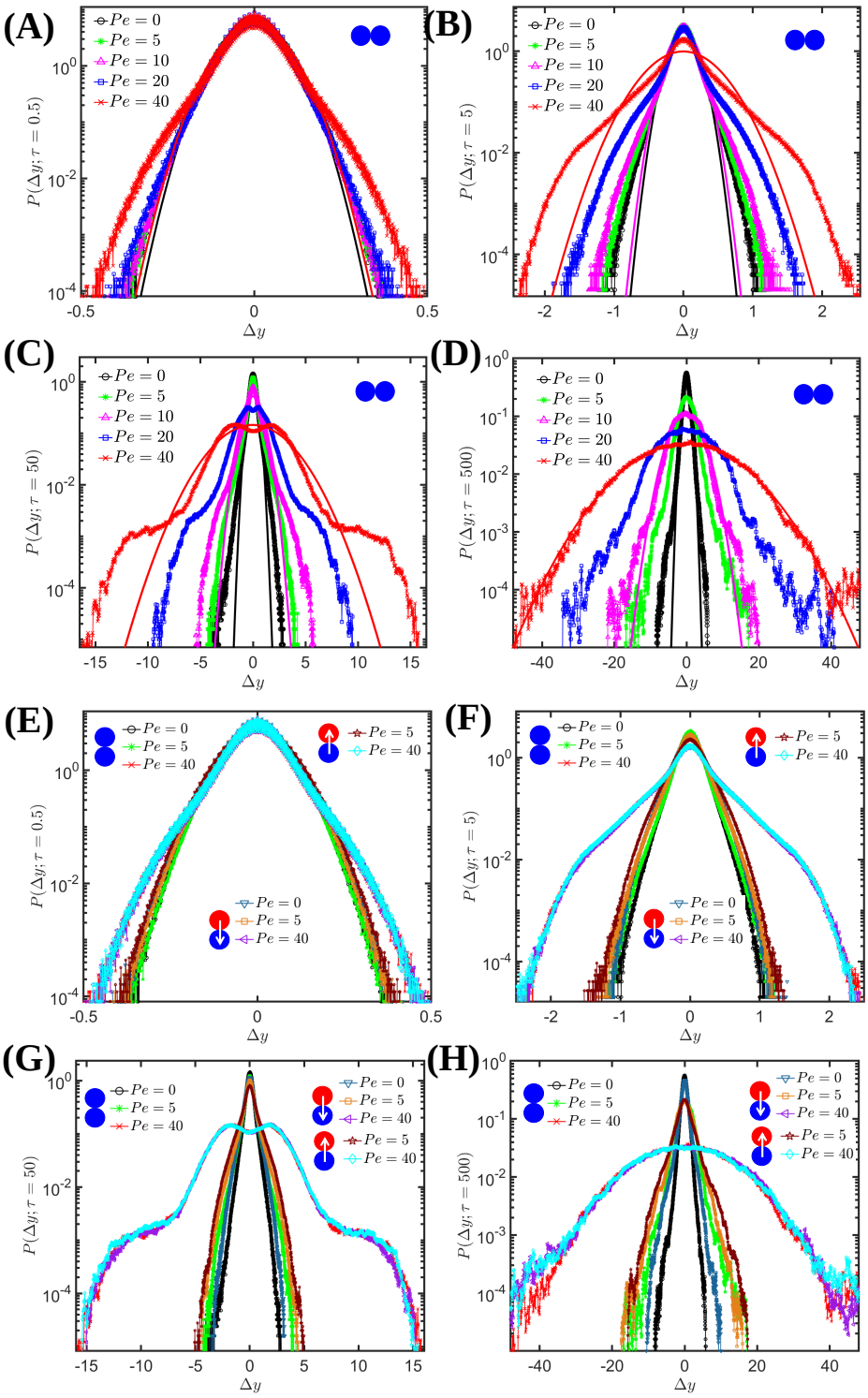

Fig. S5. Plots of P($\Delta y;\tau$) for the symmetric sticky (ϵ = 1.0) dumbbell as a function of Pe at different lag-times τ (0.5, 5, 50 and 500) (A-D). Comparison of $P(\Delta y;\tau)$ for asymmetric dumbbell with self-propulsion along the sticky ($\epsilon = 1.0$) half (arrow towards blue half), self-propulsion along the non-sticky half (arrow towards red half), and symmetric dumbbell in the polymer gel for Pe = 0, 5, and 40 at different lag-times τ (0.5, 5, 50 and 500) (E-H). The Solid lines represent the Gaussian fittings.

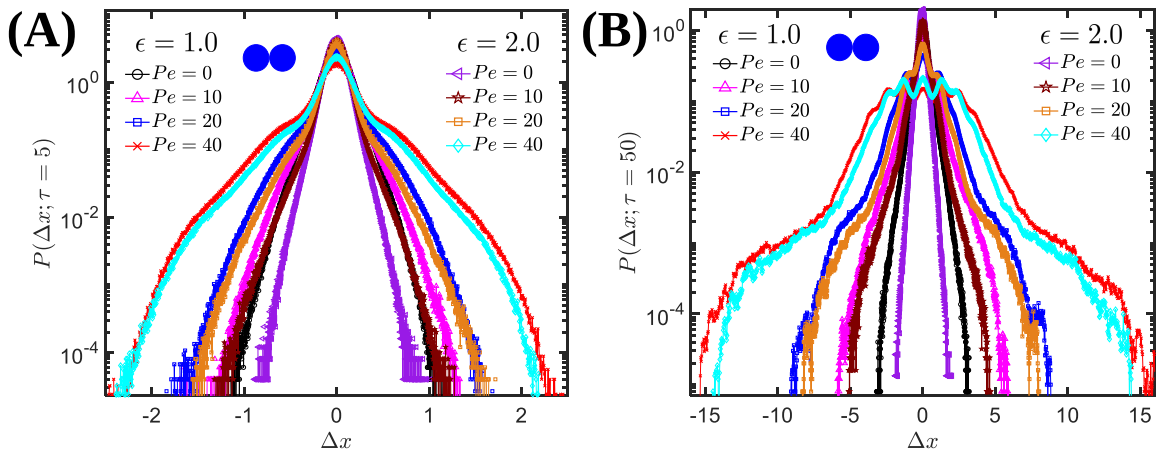

Fig. S6. $P(\Delta x; \tau)$ for the attractive symmetric dumbbell for $\epsilon = 1.0$ and $\epsilon = 2.0$ at lag-time (A) $\tau = 5$, and $\tau = 50$ for different Pe.

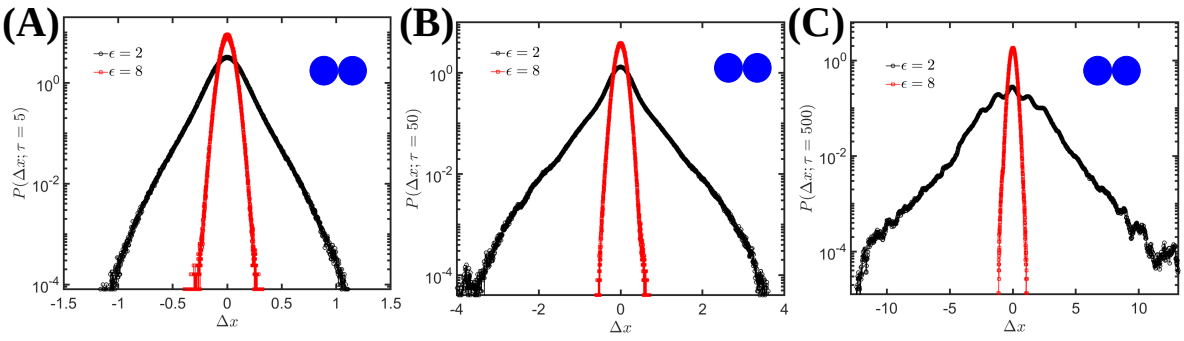

Fig. S7. $P(\Delta x; \tau)$ for the attractive symmetric dumbbell for $\epsilon = 2.0$ and $\epsilon = 8.0$ at lag-time (A) $\tau = 0.5, 5$, and $\tau = 50$ for Pe $= 5$.

Movie description

Movie_S1

Molecular dynamics simulation of the passive (Pe = 0) chemically symmetric rigid dumbbells with both the halves are sticky to the monomers of the polymer gel (green in color). It is clear from the movie that the chemically symmetric rigid dumbbells are transiently trapped inside the polymer mesh.

Movie_S2

Molecular dynamics simulation of the self-driven (Pe = 20) chemically symmetric rigid dumbbells with both the halves are sticky to the monomers of the polymer gel. One can see that the self-propulsion helps the dumbbell escape from the confined polymer mesh and cover a larger area inside the gel.

Movie_S3

Molecular dynamics simulation of the self-driven (Pe = 20) chemically asymmetric rigid dumbbells with one sticky half (blue) and the other non-sticky (red) to the monomers of the polymer gel. Here, the direction of the self-propulsion is along the sticky (blue) half, which promotes the hindered motion of dumbbells inside the gel as it moves along the sticky half.

Movie_S4

Molecular dynamics simulation of the self-driven (Pe = 20) chemically asymmetric rigid dumbbells with one half being sticky (blue) while the other half being non-sticky (red) to the monomers of the polymer gel. Here, the direction of the self-propulsion is along the non-sticky half (red), which facilitates the escape of the dumbbells as it moves along the non-sticky half inside the gel.