Supplementary Material: Demixing of active-passive binary mixture through a two-dimensional elastic meshwork

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TABLE I. Model Parameters

Parameter	**Value**
σ_{tracer}	2σ
σ_{beads}	σ
l_{mesh}	$\sigma,\ 1.5\sigma,\ 2.0\sigma,\ 2.5\sigma$
$\frac{m}{\zeta}$	10^{-2}
k_BT	1
Δt	5×10^{-3}
ϵ_{ij}	1
F_a	0, 5, 10, 15, 20, 30, 40, 50, 60, 70

I. MEAN-SQUARED DISPLACEMENT, DIFFUSION COEFFICIENT AND PERSISTENCE TIME OF A FREE ACTIVE BROWNIAN PARTICLE

To understand the dynamics and persistence time of ABPs with the mentioned parameters ($\gamma = 100,\ \sigma_{tracer} = 2\sigma$), we perform controlled simulations for free ABPs at different activity. The time-averaged mean square displacement is calculated as: $\overline{\Delta r_i^2(\tau)} = \frac{1}{T_{\max}-\tau}\int_0^{T_{\max}-\tau}[r_i(t+\tau)-r_i(t)]^2\,dt$ followed by an ensemble average over N_{trj} trajectories, defined as: $\langle\overline{\Delta r^2(\tau)}\rangle = \dfrac{1}{N_{trj}}\sum_{i=1}^{N_{trj}}\overline{\Delta r_{\rm i}{}^2(\tau)}$. A plot showing the time evolution of $\langle\overline{\Delta r^2(\tau)}\rangle$ is shown in Fig. S1 (a). The effective diffusion coefficient, D_{eff}, is calculated using the equation:

$$D_{eff} = \lim_{\tau\to\infty}\frac{\langle\overline{\Delta r^2(\tau)}\rangle}{6\tau}$$

In the presence of thermal noise, the effective diffusion coefficient of ABPs has two contributions: thermal diffusivity D_T and the convective diffusivity, such that $D_{eff} = D_T + D_{swim}$ [1]. In the dilute limit D_{swim} is given by: $D_{swim} = \frac{F_a^2 \tau_R}{3\gamma^2}$. Using this equation, the persistence time is determined from the intercept of the log-log plot of D_{swimm} versus activity which is shown in Fig. S1 (b), where Pe is defined as $Pe = \frac{F_a \sigma_{tracer}}{k_B T}$.

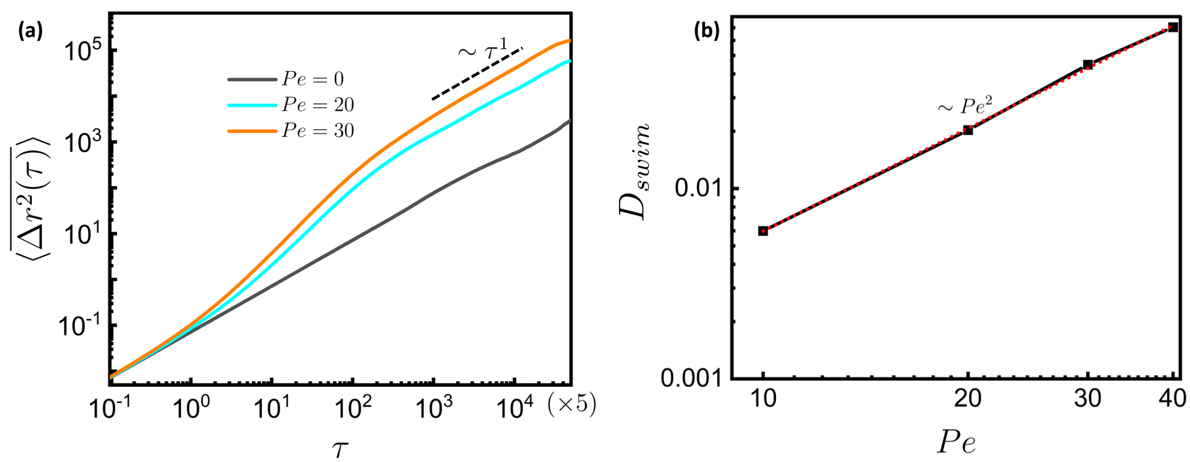

Fig. S1. Log-log plot of (a) $\langle \overline{\Delta r^2(t)} \rangle$ with time and (b) active diffusion coefficient D_{swim} with Pe, where red dotted line is the fitted Pe^2.

II. PRESSURE EXERTED ON THE BEADS OF THE MESHWORK

The pressure exerted on individual bead i_b of the meshwork (Fig. 1 (b) in the main manuscript), is defined as the trace of the stress tensor:

$$\Pi_{Mesh-bead} = -\frac{1}{3dV}(\Sigma_{xx} + \Sigma_{yy} + \Sigma_{zz}), \tag{1}$$

where dV is the Voronoi volume of the meshwork bead i_b, Σ_{xx}, Σ_{yy} and Σ_{zz} are the diagonal components of the energy tensor[2, 3]. In general, the diagonal component $\Sigma_{\alpha\alpha}$ is defined as:

$$\Sigma_{\alpha\alpha} = -[m v_\alpha v_\alpha + \frac{1}{2}\sum_{n=1}^{N_{pair}}(r_{1\alpha}F_{1\alpha} + r_{2\alpha}F_{2\alpha}) + \frac{1}{2}\sum_{n=1}^{N_{bond}}(r_{1\alpha}F_{1\alpha} + r_{2\alpha}F_{2\alpha}) + \frac{1}{3}\sum_{n=1}^{N_{angle}}(r_{1\alpha}F_{1\alpha} + r_{2\alpha}F_{2\alpha} + r_{3\alpha}F_{3\alpha})]. \quad (2)$$

The first term represents a pairwise energy contribution, where n loops over the N_{pair} neighbors of bead i_b, r_1 and r_2 are the positions of the two particles (monomers of the mesh along with the other particles in the system) involved in the pairwise interaction, and F_1 and F_2 are the forces acting on the two particles as a result of the interaction. The second and third terms represent the bond and angle contributions, respectively, with a similar form applied to the bonds and angles involving bead i_b (Fig. 1 (b) in the main manuscript). We plot the spatial distribution of pressure in Fig. S4, for different $\tilde{\sigma}$ and $Pe = 80$. To quantify the contribution of pressure from activity, we calculate a quantity χ which is defined as: $\chi = -(\langle\overline{\Pi_{Mesh-bead}(Pe)}\rangle - \langle\overline{\Pi_{Mesh-bead}(Pe=0)}\rangle)$, where $\langle\overline{\Pi_{Mesh-bead}(Pe)}\rangle = \langle\frac{1}{t_{max}-t_1}\sum_{n=t_1}^{t_{max}}\langle\Pi_{Mesh-bead}\rangle(Pe)\rangle$ represents the averaged pressure on the meshwork beads when 50% of the colloidal particles are passive and the other 50% are active. In contrast, $\langle\overline{\Pi_{Mesh-bead}(Pe=0)}\rangle = \langle\frac{1}{t_{max}-t_1}\sum_{n=t_1}^{t_{max}}\langle\Pi_{Mesh-bead}\rangle(Pe=0)\rangle$ represents the averaged pressure on the meshwork beads when all the particles are passive. This residual pressure on the meshwork at $Pe = 0$ has two contributions: one from Brownian dynamics and the other from the pressure exerted by the meshwork beads on one another, governed by their mutual interactions.

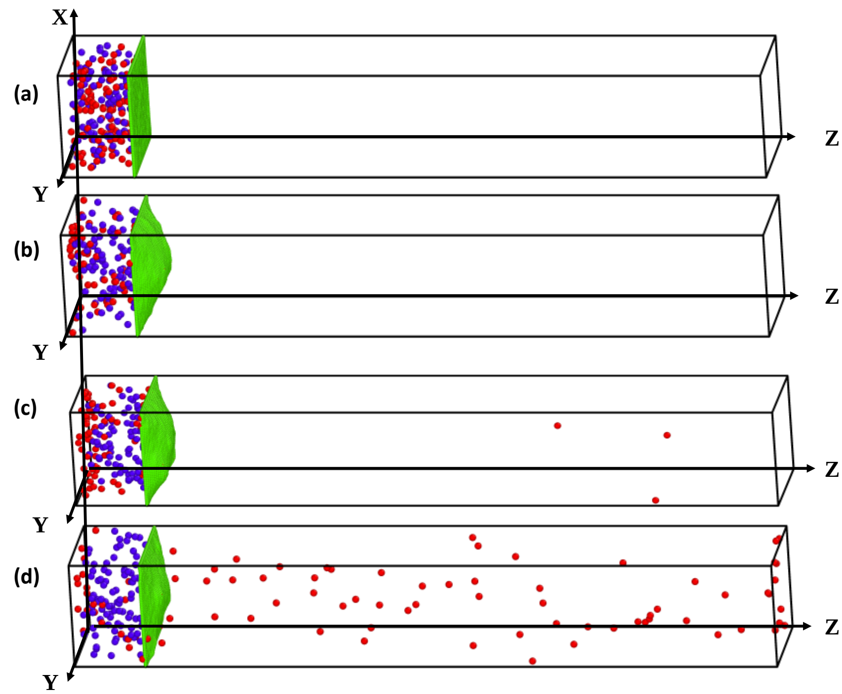

Fig. S2. Snapshots of the system with a monodisperse binary mixture of active and passive colloidal particles, allowed to pass through the meshwork, are shown as follows:(a) The initial frame, the final frame at (b) $Pe = 120$, (c) $Pe = 180$ and (d) $Pe = 220$ with $\tilde{\sigma} = 2.00$. Here, active particles are shown in red, passive particles in blue, and the meshwork beads in green.

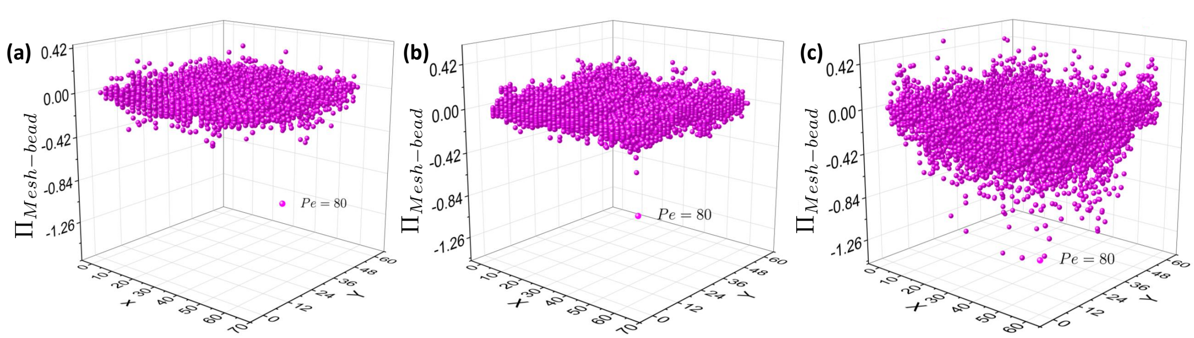

Fig. S3. Plots showing the spatial distribution of pressure on meshwork beads for $\tilde{\sigma}$: (a) 0.80, (b) 1.00, and (c) 1.33, with $K = 50$ and $Pe = 80$.

Movie description

Movie_S1

The movie demonstrates that the passive particles (blue), initially separated from the rest of the box by a two-dimensional meshwork (green) ($\tilde{\sigma} = 0.8$ and $K = 50$), are able to pass through the meshwork.

Movie_S2

The movie shows that the passive particles (blue), initially separated from the rest of the box by a two-dimensional meshwork (green) ($\tilde{\sigma} = 1.0$ and $K = 50$), are unable to pass through the meshwork.

Movie_S3

This is evident from the movie, where a 1:1 monodisperse active (red)–passive (blue) binary mixture, initially separated from the rest of the box by a two-dimensional meshwork (green) ($\tilde{\sigma} = 1.0$, $Pe = 80$, and $K = 50$), shows a significant permeation of active particles through the meshwork.

Movie_S4

A 1:1 monodisperse active (red)–passive (blue) binary mixture, initially separated from the rest of the box by a two-dimensional meshwork (green) ($\tilde{\sigma} = 1.33$, $Pe = 80$, and $K = 50$), is shown in the movie, which demonstrates that there is no significant permeation of active particles through the meshwork.

Movie_S5

In this movie, a 1:1 monodisperse binary mixture of active (red) and passive (blue) particles is initially confined within a two-dimensional meshwork (green) ($\tilde{\sigma} = 1.33$ $Pe = 120$, and $K = 50$). It is evident that the active particles primarily permeate through the meshwork.

Movie_S6

The movie illustrates the significant permeation of active particles (red) through the two-dimensional meshwork (green), which initially separates a 1:1 monodisperse binary mixture of active (red) and passive (blue) particles ($\tilde{\sigma} = 1.33$, $Pe = 80$, and $K = 20$).

[1] Y. Du, H. Jiang and Z. Hou, *Soft Matter*, 2019, **15**, 2020.

[2] A. P. Thompson, S. J. Plimpton and W. Mattson, *J. Chem. Phys.*, 2009, **131**, 154107.

[3] R. G. Winkler, A. Wysocki and G. Gompper, *Soft Matter*, 2015, **11**, 6680.