Supplementary Materials for

Emergent stereoselective interactions and self-recognition in polar chiral active ellipsoids

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(available at advances.sciencemag.org/cgi/content/full/7/9/eabd0331/DC1)

Movies S1 to S7
Supplementary Sections & Supplementary Figures

S1. Details of 3D-printing

Fig. S1. Tray with a batch of 3D printed particles. Photo Credit: Pragya Arora, JNCASR
S2. Measuring vertical and horizontal components of acceleration

![Graph showing vertical and horizontal acceleration components.](image)

**Fig. S2. Vertical and horizontal components of acceleration.** Plotted here are accelerometer readings taken at 37 Hz of the vertical and horizontal components.

S3. Imaging the particles

![Snapshot of flower shaped tray with particles.](image)

**Fig. S3. Imaging the particles.** Snapshot of the entire field of view of the flower shaped tray on top of which particles are vibrated. *Photo Credit: Pragya Arora, JNCASR*
S4. Particle Design

Fig. S4. Snapshots of 3D-printed polar and apolar ellipsoids. (A) Apolar active ellipsoids (B) Polar active ellipsoids with an asymmetry in friction coefficient $\mu$ (C) Polar active ellipsoids with an asymmetry in $\mu$ and mass $m$. (D and E) Chiral polar active ellipsoids with an asymmetry in $\mu$ and $m$ asymmetry along minor-axis. (D) Mass asymmetry due to hole. (E) Mass asymmetry achieved by hollowing one portion of ellipsoid. (A-E) Photo Credit: Pragya Arora, JNCASR

Many designs of polar and apolar ellipsoids were tested, and the design was finalized based on the nature of active dynamics observed. We started by printing uniform apolar ellipsoids with a head-tail symmetry (Fig. S4A), under vertical agitation, these ellipsoids took both forward and backward steps along the major axis with no preferential direction. Next, an asymmetry in the friction coefficient along the major axis of these ellipsoids was included to make them polar active. Thus, one end of the ellipsoid was made rougher than the other end, (see Fig. S4B) by using a property unique to the printing process and elaborated in materials and methods. This friction difference made the particles polar active with the smooth end (transparent part) as the head and rough end (white part) as the tail. These particles have a fore-aft asymmetry and are intrinsically polar active along the direction set by the asymmetry. Next, a hole was printed along the major axis towards the rough end of the particle (the tail or the trailing end) to incorporate a mass anisotropy in the design (see Fig. S4C). It was found that these ellipsoids were also self-propelled along its major axis with the hole at the trailing end, and moved faster than the earlier ellipsoids (Fig. S4B). To impart a chirality to the particle, the left-right symmetry along the propulsion direction has to be broken, even minute deviations from this symmetry alter the straight path of the particle. Thus, to design chiral particles, the
hole position was moved along the minor as well as the major axis (see Fig. S4D), resulting in an active torque in addition to the active force and rendering the particle chiral. These particles had a handedness in their motion and executed circular trajectories with an extremely large radius. Further, to tune the radii of these particles, we hollowed out one side of the ellipsoid along the longitudinal cross-section (see Fig. S4E). The white region on the right side of the major axis shown in Fig. S4E is the hollowed-out region. The volume of this hollowed-out portion was changed in other ellipsoids to tune the active torque, and thus this was the control parameter to tune chirality.

S5. Spread in particle mass for a given $\Delta m_{LR}$ value

By changing the volume of hollowed out portion we tuned the extent of left-right mass asymmetry $\Delta m_{LR}$. Further, the print process was optimized to ensure that the spread in the particle mass $M$ for a given $\Delta m_{LR}$ was quite narrow (Fig. S5). In-order to obtain the error bars, we weighed 20 different particles of a batch with a given $\Delta m_{LR}$ value.

![Graph showing the mass of each particle $m$ (in gram) versus the extent of left-right mass asymmetry $\Delta m_{LR}$. The y-axis error bars represent the standard deviation of the mean value of $m$ obtained by weighing 20 different particles of the same batch for a given $\Delta m_{LR}$ value.](image_url)
S6. Orientational mean-squared displacement of monomer and mover

We quantified the orientational mean-squared displacement (MSD), in the dilute limit for movers and monomers of C$_2$ ellipsoids.

\[
\langle \Delta \theta^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \Delta \theta_i(t)^2
\]

Here, \( \langle \rangle \) denotes average over the number of dimers \( N \), and \( \theta_j(t) \) is the orientation of the \( j^{th} \) ellipsoid, \( t_0 \) is the lag time and \( \Delta \theta_i(t) \) is the orientational displacement of the particles over time \( t \).

Fig. S6. Orientational mean-squared displacement. \( \langle \Delta r^2 \rangle \) versus time of monomer (blue \( \triangle \)) and mover (red \( \square \)) of C$_2$ ellipsoids.
S7. Translational mean-squared displacement of spinner and mover and spinner dynamics

We quantified the translational mean-squared displacement (MSD), in the dilute limit for movers and spinners of C$_2$ ellipsoids.

\[ \langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_{j=1}^{N} \left[ (x_j(t + t_0) - x_j(t))^2 + (y_j(t + t_0) - y_j(t))^2 \right] \]  

(2)

Here, \( \langle \rangle \) denotes average over the number of dimers \( N \), and \( x_j(t) \) and \( y_j(t) \) are the coordinates of center of mass of the \( j^{th} \) dimer, \( t_0 \) is the lag time and \( \Delta r \) is the displacement of the particles over time \( t \).

![Graph showing the translational mean-squared displacement of dimers](image)

Fig. S7. Translational mean-squared displacement of dimers. \( \langle \Delta r^2 \rangle \) versus time of the spinner (black \( \bigcirc \)) and mover (red \( \square \)) of C$_2$ ellipsoids.

We have also calculated the angular frequency for the spinner and the individual monomer and these are found to be 4 rad/s and 12 rad/s, respectively. This is not a simple combination of the individual ellipsoids.
Fig. S8. Mover lifetimes of polar chiral active ellipsoids. (A) Probability distribution of mover lifetimes. The average lifetime $\tau_{\text{mov}}$ is shown by dashed vertical lines. (B) Mover lifetimes of $C_1C_1$, $C_2C_2$, $C_3C_3$, $C_4C_4$, $C_5C_5$ and $C_6C_6$ dimer configurations. The error bars represent standard deviation of the mean associated with the exponential fitting of the probability distribution.
Fig. S9. Phase diagram in $(\chi, \phi)$ plane. Snapshots of the experiment at various $\phi$ for $\chi = 0, \chi = 0.5$ and $\chi = 1$. Photo Credit: Pragya Arora, JNCASR.
S9. Phase diagram in $(\chi, \phi)$ plane

The phase diagram shows the snapshots of the experiment for $\phi$ ranging from 0.2 to 0.81 at $\chi = 0$, $\chi = 0.5$ and $\chi = 1$ respectively. Note the formation of dynamic clusters for $\phi > 0.2$.

Fig. S10. Orientational colour map Zoomed in region of the experimental snapshots at $\phi=0.64$ for $\chi = 1$. Major-axis of ellipsoids are colored according to their orientation. We do not observe large-range orientational correlations and collective rearrangements. Photo Credit: Pragya Arora, JNCASR.
S10. Relaxation dynamics of polar chiral active liquids

We have quantified the orientational relaxation dynamics using the $n^{th}$ order orientation correlation function $L_n(t)$ defined as:

$$L_n(t) = \frac{1}{N} \sum_{j=1}^{N} \cos n (\Delta \theta_j(t))$$ (3)

Here, $N$ is the total number of particles, $\theta_j(t)$ is the orientation of the $j^{th}$ ellipsoid at time $t$. The $L_1(t)$ correlation function was used for further analysis.

The translational dynamics was quantified using the self-intermediate scattering function $F_s(q, t)$ defined as:

$$F_s(q, t) = \frac{1}{N} \sum_{j=1}^{N} e^{i q \cdot \Delta r_j(t)}$$ (4)

Here $q$ is the wave vector, $N$ is the total number of particles, $r_j(t)$ is the position of the $j^{th}$ ellipsoid at time $t$.

We defined the orientational and translational relaxation times, $\tau_R^a$ and $\tau_T^a$, respectively, as the time at which the corresponding correlation functions decay to 0.1.

The variation of $L_n(t)$ and $F_s(q, t)$ as a function of $\phi$ for $\chi = 0$, $\chi = 0.5$ and $\chi = 1$ are shown in Fig. S11.
Fig. S11. Translational and orientational relaxation dynamics of polar chiral active liquids. (A, C, E) Self intermediate scattering function $F_s(q = 1.4\text{mm}^{-1}, t)$ for various $\phi$'s for (A) $\chi = 0$, (C) $\chi = 0.5$ and (E) $\chi = 1$. (B, D, E) Dynamic orientational correlation function $L_1(t)$ versus time for various $\phi$'s for (B) $\chi = 0$, (D) $\chi = 0.5$ and (F) $\chi = 1$. 
Fig. S12. Translational and orientational relaxation dynamics of enantiopure liquid. $\tau_T^T$ and $\tau_R^R$ versus $\phi$ for $\chi = 1$.

S11. Quantifying dynamical heterogeneity

To quantify the heterogeneities the first step is to determine the deviations from Gaussian dynamics using the non-Gaussian parameter $\alpha_2$. Non Gaussian parameter $\alpha_2$, is simply the kurtosis of the distribution of particle displacements and quantifies the deviations from Gaussian dynamics.

$$\alpha_2 = \frac{(\Delta r^4(t))}{2(\Delta r^2(t))^2} - 1,$$

Here $\Delta r$ is the particle displacement over time $t$. This function has a peak value close to the cage rearrangement time $t^*$, where the dynamics is maximally heterogeneous. Fig. S13 shows non-Gaussian parameter $\alpha_2^T$ at various $\chi$’s for $\phi = 0.72$ for one experimental realization.
Fig. S13. Quantifying dynamical heterogeneity. The time dependence of translational non-Gaussian parameter $\alpha_T^2$ at different $\chi$ values for $\phi = 0.72$. The time corresponding to the peak value of $\alpha_T^2$ is $t^\star$.

Supplementary Movies

Movie S1. Tunable chiral active motion in vertically vibrated 3D-printed ellipsoids

Movies showing motion of C$_2$, C$_4$ and C$_6$ polar chiral active ellipsoids under vertical vibration. The particles execute noisy circular trajectories with a well-defined $R$ and $\omega$. The movies are 1.5X faster than real-time.

Movie S2. Active mover

Movie showing a representative active ‘mover’ mode of C$_2$ ellipsoids. The mover is composed of a dextro- (+) and levogyre (-) monomer. The motion of the mover is similar to an achiral polar active particle. The movie is 1.5X faster than real-time.

Movie S3. Active spinner

Movie showing a representative active ‘spinner’ mode of C$_2$ ellipsoids. The spinner is made of two dextro-(+) monomers, the spinner has a net clockwise (+) motion and is localized in space. The movie is 1.5X faster than real-time.
Movie S4. Mover lifetime as a function of increasing radii

Movies showing dynamics in racemic mixtures for each type of ellipsoid (C_1 to C_6). As $R$ increases from C_1 to C_6, the mover lifetime decreases. The movies are 1.5X faster than real-time.

Movie S5. Dynamics of racemic mixture of C_2 and C_4 ellipsoids

Movie showing a 1:1 mixture of individually racemic C_2 and C_4 ellipsoids at $\phi = 0.10$. The C_4 ellipsoids have a black dot on them to distinguish them from C_2 ellipsoids. The movie is 1.5X faster than real-time.

Movie S6. Self-recognition in polar chiral active ellipsoids

Movie showing three mover configuration - C_2 C_2, C_2 C_4 and C_4 C_4. The C_2 and C_4 ellipsoids have a blue and red dot marked on them respectively. The movers made of like particles were longer-lived in comparison to those made of unlike ones. The movie is 3.75X faster than real-time.

Movie S7. Dynamics of polar chiral active liquids as a function of net chirality

First row: Movies showing raw data of chiral active liquids of C_2 at $\phi = 0.84$ as a function of net chirality. Second row: Displacement maps for chiral ellipsoids at $\phi = 0.84$ and over a time corresponding to $7t^*$. Red color represents high particle overlaps and blue represents poor overlaps. The movies are 10X faster than real-time.