Supplementary Material for

Active transformations of topological structures in light-driven nematic disclination networks

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This PDF file includes:

- Materials and Methods
- Fig. S1-S17
- Supplementary text
- Captions for Movies S1 to S6

Other Supplementary Materials for this manuscript includes the following:

- Movies S1 to S6
Materials and methods

Fig. S1. Molecular structure of materials. Molecular structure of amphiphile comprised of fatty acid C5 conjugated to BODIPY (BODIPY-C5) (A), nematic liquid crystal 5CB (B), photosensitive azo-dye SD1 (C) and liquid crystal monomer RM257 (D).
Fig. S2. Schematic of patterned substrate preparation. (A) Photo-patterning setup based on projector display; (B) Director field of topological defect +1 with pure bend; (C) The pattern is divided into 36 segments and each segment has 10° opening angle; (D) The starting segment in the black background; The linearly polarized light will go through the white segment; After the first exposure is finished, the second segment will be projected to the substrate coated with SD1; The exposures will go on and go forth until the $2\pi$ rotation is completed.
Fig. S3. Patterned topological defects. (A) Director field of +1 defect with pure bend; (B) Polarizing microscope texture of the circular pattern designed in (A); (C) Polarizing microscope image of circular pattern with red plate engaged; (D)-(F) Designed and produced +1/2 defect; (G)-(I) Designed and produced 2D lattice of (+1, -1) defects; (J)-(L) Designed and produced 2D lattice of (+1/2, -1/2) defects; Scale bar is 50μm.
**Supplementary text**

Following the numerical formula stated in the main text, we performed finite-difference based numerical simulations on different patterns used in experiments and we analyzed the transformations between different topological structures.

(1) Topological transformation in a 2D lattice of (+1/2,-1/2) topological defects

![Diagram](image)

**Fig. S4** An illustration for vector $T$, $Ω$, $m$, $N$, $e_1$, $e_2$ and angle $α$, $β$, $γ$.

In order to understand the spatiotemporal dynamics of 3D active nematic disclinations in Fig. 1, continuum simulations are conducted. At the initial state, the angle $γ$ between $N$ and $Ω$ is $π/2$, implying a wedge-twist type, fig. S5A. As shown in Fig. 1, as the top substrate alignment rotates, angle $γ$ goes down firstly and this decrease gradually turns the curve towards a pure-twist type. Before that happens, defects merge, which leads to another increase in angle $γ$. For the
topological transformation, it is shown that topological structure transforms from wedge-twist-I with $\alpha=\pi/2$, $\gamma=\pi/2$, fig. S5A, to wedge-twist-II profile with $\alpha=-\pi/2$, $\gamma=\pi/2$, fig. S5B.

Fig. S5. Topological transformation from wedge-twist-I (A) profile to wedge-twist-II (B) profile after light irradiation on the 2D lattice of (-1/2, 1/2) topological defects; (C) Temporal change of orientation angles of disclination lines at +1/2 and -1/2 respectively;
For twist angle analysis, we look at defect line colored with angle $\beta$, the difference angle between tangent $\mathbf{T}$ and rotation vector $\mathbf{\Omega}$, shown in Fig. S6. The defect line is close to the bottom substrate with the shape of a shallow arc. At two ends of the curve, $\beta$ is approximately $0.4\pi$ (near $+1/2$ charge) and $0.6\pi$ (near $-1/2$ charge); in the middle of the curve, $\beta = 0.5\pi$ and refers to a tangential twist winding profile. $\mathbf{\Omega}$ is constant and thus normal to the curve normal $\mathbf{N}$. Also, along the defect curve, $\beta \in [0.4\pi, 0.6\pi] \subset [0, \pi]$, so defect structure can be regarded as a part of a wedge twist loop in fig. S4.

![Twist angle $\beta$ analysis along the disclination line for wedge-twist profile.](image)

**Fig. S6.** Twist angle $\beta$ analysis along the disclination line for wedge-twist profile. Twist angle of a defect line connecting $+1/2$ and $-1/2$ point defects (pattern in Fig. 1). Insets are three local director profiles with two at the ends of the curve and one in the middle of it.

(2) Topological transformation in 2D lattice of (-1,+1) topological defects

When the pattern is irradiated by light, it is shown that topological structure transforms from wedge-twist-II with $\alpha = -\pi/2$, $\gamma = \pi/2$, Fig. S7A, to the same wedge-twist-II profile with $\alpha = -\pi/2$, $\gamma = \pi/2$, Fig. S7B, after the recombination events of disclination lines.
Fig. S7. (A)-(B) Topological transformation from wedge-twist-II to wedge-twist-II during light irradiation on the 2D lattice of (+1, -1) topological defects; (C) Orientational changes of disclination lines at +1 and -1 respectively.
Topological transformations in a 2D lattice of (-1/2,+1/2) defects with dipoles in the same direction

If the pattern shown in Fig. 3A is irradiated by the light, the topological structure from wedge-twist-I with $\alpha = \pi/2$, $\gamma = \pi/2$, fig. S8A, transforms into two different topological structures. One profile is wedge-twist-II with $\alpha = -\pi/2$, $\gamma = \pi/2$, fig. S8B, and the other one is a tangential-twist-II profile with $\alpha = -\pi/2$, $\gamma = 0$, fig. S8C.

**Fig. S8.** Topological transformation from wedge-twist-I to wedge-twist-II and tangential-twist-II profiles during light irradiation on the 2D lattice of (+1/2, -1/2) topological defects with same-direction dipoles.
The defect line shown in fig. S8C at the region between (+1/2, -1/2) defect pairs only has $\beta = \pi/2$ profile throughout, fig. S9.

![Image](image_url)

**Fig. S9. Local twist profile.** Twist angle of the defect line formed at the region between (+1/2, -1/2) defect pairs (pattern in Fig. 3M). This curve has constant local director profile.

(4) Topological transformation of disclination lines with pure-twist profiles

Disclination lines with pure-twist profiles are formed in the pattern with alternating splay and bend distortions, Fig. 5. Upon light irradiation, the topological structure transforms from tangential-twist-I with $\alpha = \pi/2$, $\gamma = 0$, fig. S10A to tangential-twist-II profile with $\alpha = -\pi/2$, $\gamma = 0$, fig. S10C.

![Image](image_url)

**Fig. S10.** Topological transformation from tangential-twist-I(A) to tangential-twist-II(C) profile on the pattern with alternating splay and bend regions; (B) Temporal displacement of disclination lines.
(5) Topological transformations of disclination loops with pure-twist profiles

Figure S11 is the defect loop in Fig. 6. In Fig. S11A, top substrate director is at (1, 0, 0) and bottom substrate director is at (0, 1, 0).

![Diagram of disclination loop](image)

**Fig. S11. Angle analysis for pure-twist loop.** Pure-twist loop characterization (when top substrate director is along x axis and local direction of bottom substrate is along y axis, see Fig. 6): (A) distribution of angle $\beta$ between curve tangent $T$ and rotation vector $\Omega$; (B) Offset angle $\alpha$ along defect loop, represented by $\sin(\alpha)$.

(6) Elastic energy analysis for of (+1/2, -1/2) topological defect pattern

In Fig.1P, note that point M has a slightly lower total energy than point I due to the inequality of the four elastic constants of 5CB. We also tried to simulate the (+1/2, −1/2) cell using one elastic constant assumption ($K_1=K_2=K_3=K_{24}$), see Fig.S12 below. Compared with Fig. 1P, initial state energy and final state energy under one constant assumption are closer. Therefore, we concluded that elastic constant difference is the main cause of energy difference.

Notably, there is still a tiny insignificant difference between initial and final state in Fig.S12, and this comes from elastic energy composition difference: wedge-twist I structure resides in the splay
region (of bottom pattern); at the final state, wedge-twist II is anchored in the bend region. A comparison of splay, twist and bend energy variation by one-constant approach is shown in Fig.S13.

Twist energy at state $\varphi = 0$ and $\varphi = \pi/2$ are identical; and splay energy is the lowest of the three at $\varphi = 0$ while $\varphi = \pi/2$ state imposes a lower bend energy.

**Fig. S12** Energy changes with angle $\varphi$ by one-constant assumption. Total energy is decomposed into its two main parts, Landau-de Gennes energy and elastic energy. This shows clearly that the difference comes from elastic energy.
Fig. S13 Normalized splay, twist and bend energy variation (divided by the largest value) with angle \( \varphi \) by one-constant assumption.

(7) Orthonormal frame \( \mathbf{F} \) defined in disclination loop

Figure S14 shows simulation result of the middle plane director outside the disclination loop in Fig. 6. To record loop topology, we use an orthonormal frame \( \mathbf{F} = \{ \Omega, \mathbf{n}_{\text{out}}, \mathbf{n}_{\text{in}} \} \). \( \Omega \) (rotation vector of local profile) and \( \mathbf{n}_{\text{out}} \) (director outside the loop, blue line director in Fig. S14) are uniform in the loop. Therefore, our loops all have topological index \( v = 0 \), and therefore neutral and unlinked (30).
Fig. S14 Middle plane director details in simulation of the pattern in Fig. 6, showing inner director and outer director ($n_{\text{out}}$) are uniform.

(8) Protocol for changing $Q_{\text{surf}}$ in simulations

In our simulation, we have assumed that $Q_{\text{surf}}$ of the top surface (where there is no pattern) changes continuously from one preferred direction to another, represented by a continuous change of angle $\phi$ (see Fig. 11-M).

To justify our choice of $Q_{\text{surf}}$, we also tried a sudden change of $Q_{\text{surf}}$. Fig. S15 gives a few simulation snapshots of the system relaxation for a sudden change of $Q_{\text{surf}}$ from $0^\circ$ (initial) to $90^\circ$ (final). This choice of $Q_{\text{surf}}$ is unable to reproduce experimental observations. Therefore, the current approach matches the experiment well and is implemented throughout the manuscript.
Fig. S15 The comparison between two ways of changing $Q_{\text{surf}}$: (A), discrete change; (B), continuous change (current approach); (C), experiment results.

To ensure the continuous change, the simulation is run with a total time step of $T = 250000$, during which the rotation angle is linearly varied by $90^\circ$ between the initial and the final state. Therefore, in each time step of the simulation, the angle is increased by $\Delta \varphi \approx 6.28 \times 10^{-6}$. We have chosen such a small increment of angle to ensure that the system is evolving quasi-statically. To verify, we have compared different numbers of divisions (total time step $T$). The comparison between $T = 250000$ and $T = 500000$ (and $\Delta \varphi \approx 3.14 \times 10^{-6}$) for 2D lattice of $(+\frac{1}{2}, -\frac{1}{2})$ pattern (see Fig. S16) is shown. Two curves are almost identical with the same features realized (bend, split and reconnect of disclination lines).
Fig. S16 The comparison between $T=250000$ and $T=500000$.

In addition, after the initial conditions applied (0-degree anchoring angle on the top substrate, patterned bottom substrate and random director for the bulk points), we allowed 10000-time steps for the system to relax (Fig. S17), which meets the criteria of $(Q_{i+1} - Q_i)^2 < 1e-27$ and makes sure that we started rotation from an equilibrated state. After that, we applied the 250000 rotation steps to the equilibrated system, and the linear variation of angle is performed.

Fig. S17 Initial relaxation process before applying anchoring rotation.
Supplementary Movies

Supplementary Movie S1: Experiment and simulation of topological transformation in 2D lattice of +1/2 and -1/2 defects. The bottom substrate is designed with a 2D lattice of +1/2 and -1/2 topological defects and the top substrate has a uniform alignment. Under the light irradiation, the wedge-twist-I profile is transformed into a wedge-twist-II configuration. The numerical simulations agree with the experimental results. The video is recorded at 20 fps; playback rate is 100 fps.

Supplementary Movie S2: Experiment and simulation of topological reconfiguration in 2D lattice of +1 and -1 defects. The topological pattern adopts a 2D lattice of +1 and -1 defects. The disclination networks go through the bend, merge and split events, but the topological structures are transformed from wedge-twist-II to the same wedge-twist-II profile. The numerical simulations agree with the experimental results. The video is recorded at 20 fps; playback rate is 100 fps.

Supplementary Movie S3: Experiment and simulation of topological transformation from wedge-twist profile to pure-twist structure. The disclination networks are formed by using a topological pattern with a 2D lattice of +1/2 and -1/2 defects with dipoles pointing the same direction. Upon light irradiation, the wedge-twist-I profile can be transformed into a wedge-twist-II profile and a separate tangential-twist-II structure. The numerical simulations agree with the experimental results. The video is recorded at 20 fps; playback rate is 100 fps.

Supplementary Movie S4: Experiment and simulation of topological transformation between pure-twist profiles in disclination lines. The disclination lines are formed by using alternating splay-bend distortions. Upon light irradiation, the disclination lines are shifted along -y-axis and
the topological structure is transformed from tangential-twist-I to tangential-twist-II profile. The numerical simulations agree with the experimental results. The video is recorded at 20 fps; playback rate is 100 fps.

**Supplementary Movie S5: Experiment and simulation of topological transformation between pure-twist profiles in disclination loops.** The disclination loops are formed by using a pattern with a continuous change of director field along the radial direction. Upon light irradiation, the disclination lines shrink along the radial direction and the topological structure is locally transformed between pure-twist-I to pure-twist-II profiles. The numerical simulations agree with the experimental results, demonstrating that at an initial state, topological structures transform from tangential-twist-I to tangential-twist-II through an intermediate state of radial-twist profile along the loop. The loops shrink during the reconfiguration process as local twist profiles rotating along the loop with a continuous transformation of tangential twist and radial twist profiles following the loop. The video is recorded at 20 fps; playback rate is 100 fps.

**Supplementary Movie S6: Continuously and discretely changing Q_{surf} in 2D lattice of +1/2 and -1/2 defects.** Throughout the simulation implement, Q_{surf} changes continuously from one preferred direction to another. To justify our choice of Q_{surf}, we also tried a sudden change of Q_{surf} from 0° (initial) to 90° (final).