Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Materials for
Emergent topological phenomena in active polymeric fluids

Raj Kumar Manna[1] and P. B. Sunil Kumar[1, 2]

[1] *Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India*
[2] *Department of Physics, Indian Institute of Technology Palakkad, Palakkad 678557, India*

I. GEOMETRIC MEASURES OF ENTANGLEMENT

We characterize the entanglement of active polymers by computing linking number, average crossing number and writhing number. The linking number of two polymers C_1 and C_2, whose arch-length parametrization are $\boldsymbol{\gamma}_1(t)$ and $\boldsymbol{\gamma}_2(s)$, is defined as [1]

$$Ln = \frac{1}{4\pi}\int_{C_1}\int_{C_2}\frac{(\dot{\boldsymbol{\gamma}}_1(t)\times\dot{\boldsymbol{\gamma}}_2(s))\cdot(\boldsymbol{\gamma}_1(t)-\boldsymbol{\gamma}_2(s))}{|\boldsymbol{\gamma}_1(t)-\boldsymbol{\gamma}_2(s)|^3}dt\,ds$$

The average crossing number of a polymers C , whose arch-length parametrization is $\boldsymbol{\gamma}(t)$, is defined as

$$Cn = \frac{1}{4\pi}\int_{C}\int_{C}\frac{|(\dot{\boldsymbol{\gamma}}(t)\times\dot{\boldsymbol{\gamma}}(s))\cdot(\boldsymbol{\gamma}(t)-\boldsymbol{\gamma}(s))|}{|\boldsymbol{\gamma}(t)-\boldsymbol{\gamma}(s)|^3}dt\,ds$$

The Cn for N segments of the curve C can be calculated as [2]

$$Cn = 2\sum_{i=2}^{N}\sum_{j<i}^{N}\frac{\Omega_{ij}}{4\pi}$$

where $\Omega_{ij}/4\pi$ is the Gauss integral along the segments i, j. If position vectors of the beginning and end point of i-th segment are $\mathbf{r}_1$ and $\mathbf{r}_2$ and the beginning and end point for the j-th segment are $\mathbf{r}_3$ and $\mathbf{r}_4$, then Gauss integral between the segments i and j is given by

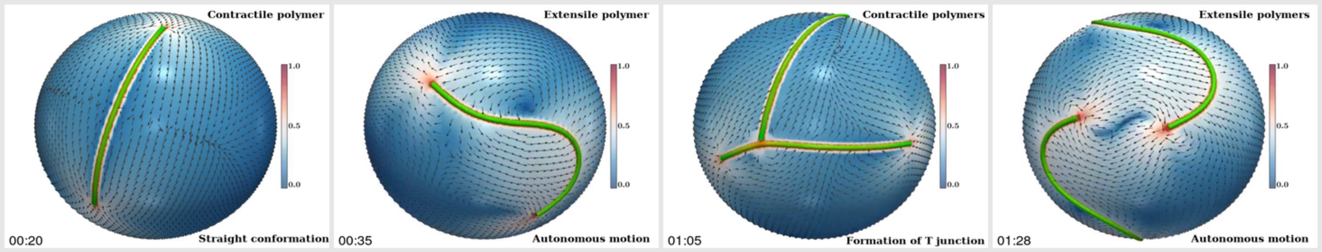
$$\Omega_{ij} = \arcsin(\mathbf{n}_1\cdot\mathbf{n}_2)+\arcsin(\mathbf{n}_2\cdot\mathbf{n}_3)+\arcsin(\mathbf{n}_3\cdot\mathbf{n}_4)+\arcsin(\mathbf{n}_4\cdot\mathbf{n}_1)$$

Here, the vectors $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ and $\mathbf{n}_4$ are defined as

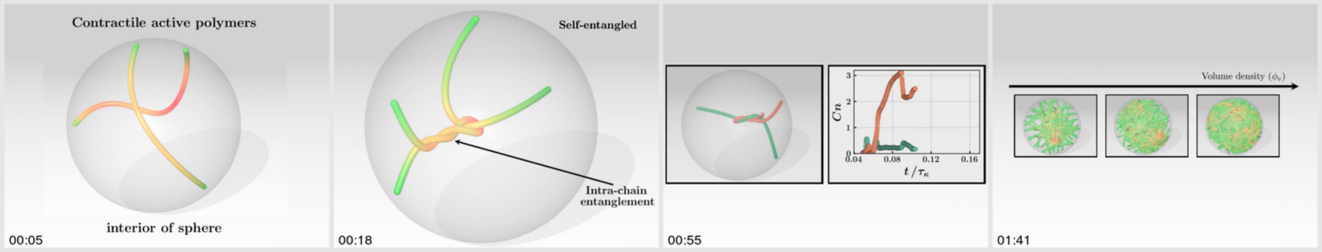
$$\mathbf{n}_1 = \frac{\mathbf{r}_{13}\times\mathbf{r}_{14}}{|\mathbf{r}_{13}\times\mathbf{r}_{14}|}, \qquad \mathbf{n}_2 = \frac{\mathbf{r}_{14}\times\mathbf{r}_{24}}{|\mathbf{r}_{14}\times\mathbf{r}_{24}|},$$
$$\mathbf{n}_3 = \frac{\mathbf{r}_{24}\times\mathbf{r}_{23}}{|\mathbf{r}_{24}\times\mathbf{r}_{23}|}, \qquad \mathbf{n}_4 = \frac{\mathbf{r}_{23}\times\mathbf{r}_{13}}{|\mathbf{r}_{23}\times\mathbf{r}_{13}|}$$

where $\mathbf{r}_{\alpha\beta} = \mathbf{r}_\beta - \mathbf{r}_\alpha$. The average linking number $\langle Ln\rangle$ is obtained by computing averages over all possible pairs of chains.

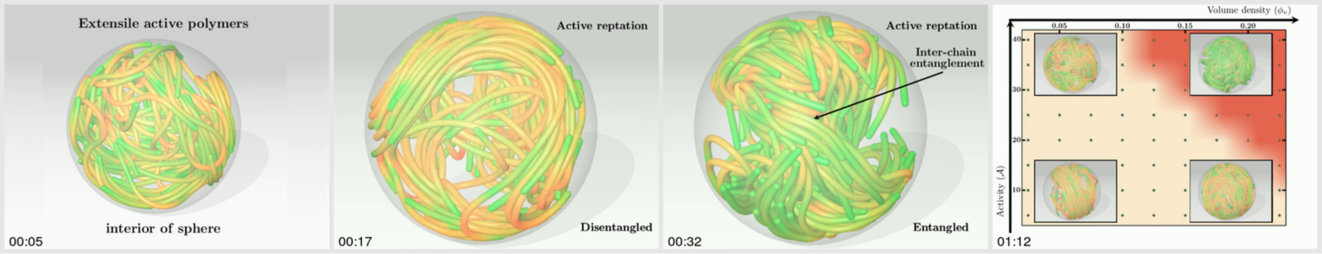
II. SUPPLEMENTARY MOVIES



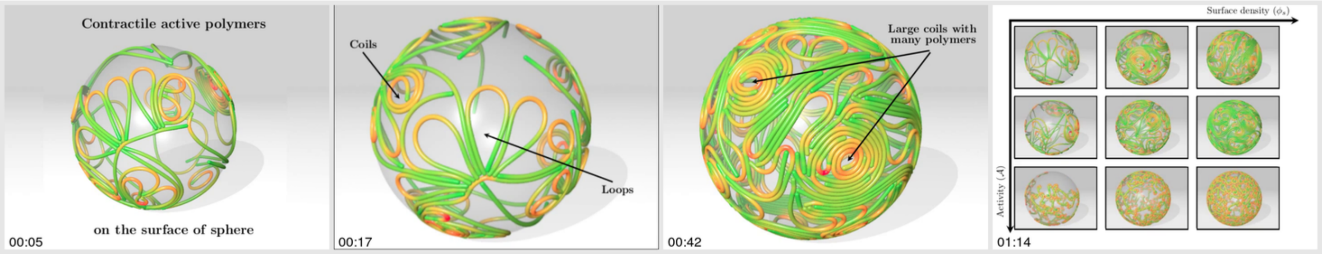
Movie S1. Fluid flows produced by active polymers. Movie S1 describes active fluid flows produced by extensile and contractile polymers on the surface of confining sphere.



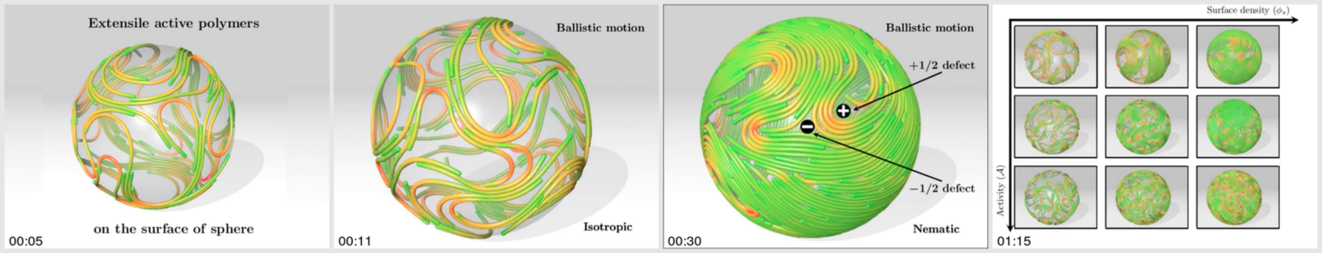
Movie S2. Contractile active polymers in volume confinement. Movie S2 describes the temporal dynamics of the contractile active polymers in the interior of volume confinement.



Movie S3. Extensile active polymers in volume confinement. Movie S3 describes the temporal dynamics of the extensile active polymers in the interior of volume confinement.



Movie S4. Contractile active polymers in surface confinement. Movie S4 describes the temporal dynamics of the contractile active polymers in the surface confinement.



Movie S5. Extensile active polymers in surface confinement. Movie S5 describes the temporal dynamics of the extensile active polymers in the surface confinement.

III. SUPPLIMENTARY FIGURES

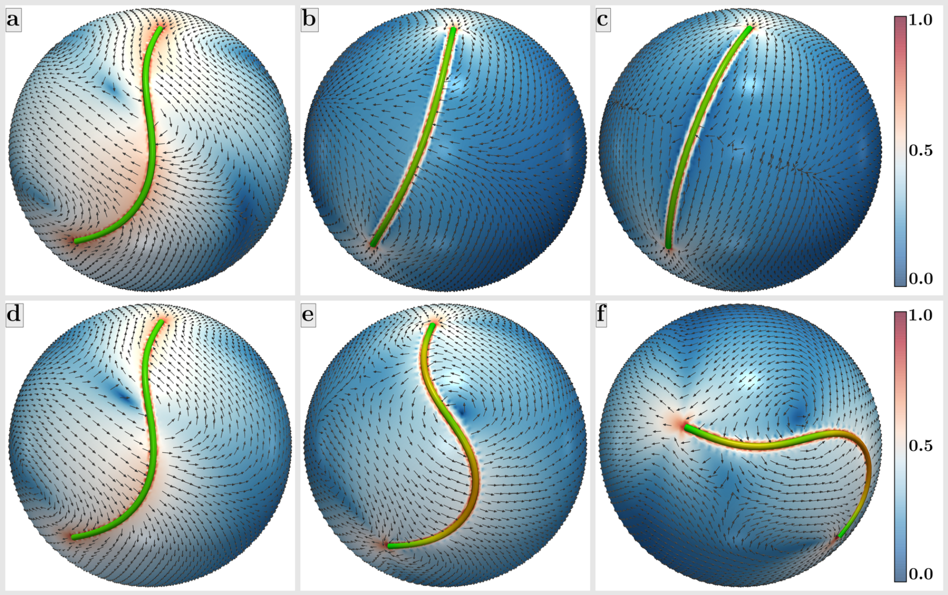


Figure S1. Fluid flows produced by a single contractile (top panel) and extensile (bottom panel) polymer on the surface of a sphere. Fluid flows are projected on the surface of the confining sphere, coloured by the logarithm of the magnitude of fluid velocity normalised by its maximum. The activity number, $\mathcal{A}$, for top and bottom panels are −30 and 30 respectively.

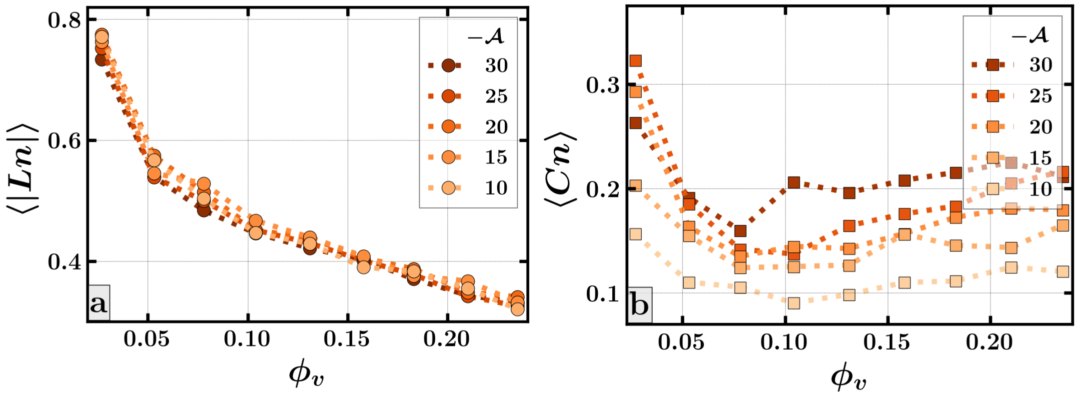


Figure S2. The average crossing number $\langle Cn\rangle$ and average linking number $\langle|Ln|\rangle$ of contractile polymers in volume confinement as a function of volume fraction for different activities.

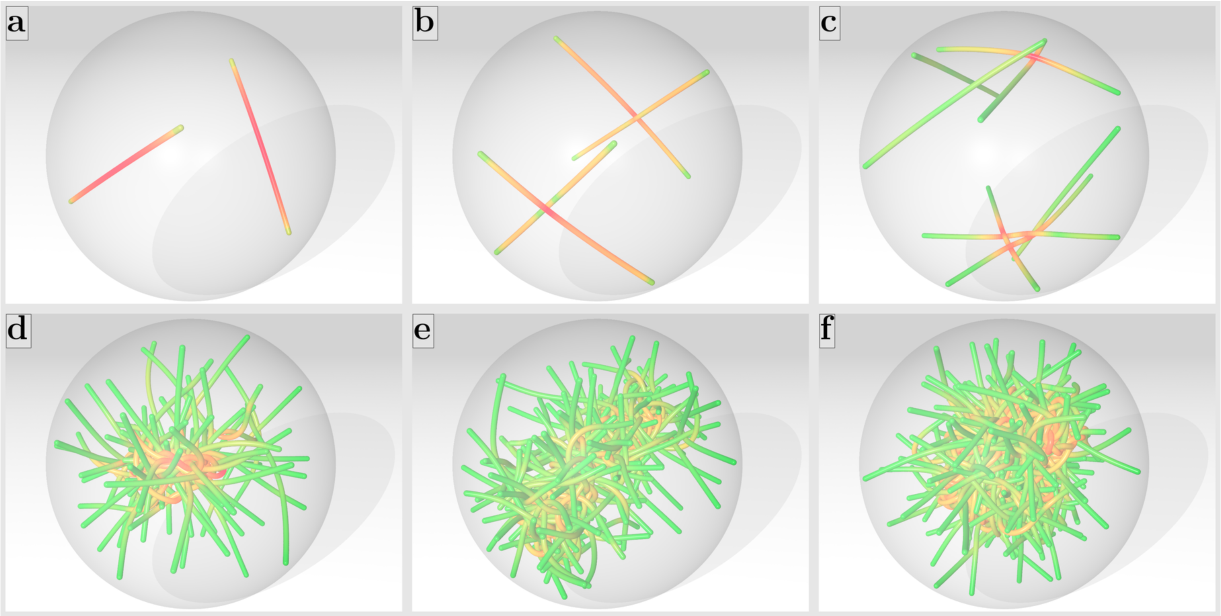


Figure S3. Contractile active polymers in volume confinement with confinement diameter larger than the polymer length. At low volume fractions, polymers in the unentangled state (a-c) but form entangled state at higher volume fraction (d-f). The activity number, $\mathcal{A}$, for all the conformations is -30.

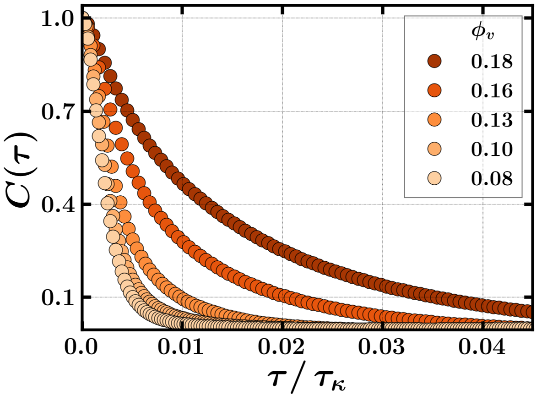


Figure S4. The autocorrelation, $C(\tau)$, of the distance between monomer pairs belonging to different extensile polymers for different volume fractions (ϕ_v), plotted in units of the bending relaxation time τ_κ at activity $\mathcal{A} = 30$.

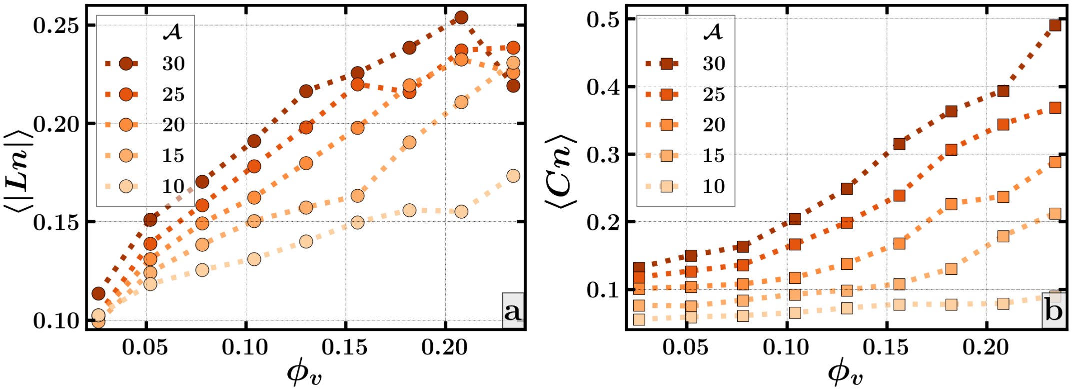


Figure S5. The average linking number $\langle Ln\rangle$ and average crossing number $\langle Cn\rangle$ of extensile polymers in volume confinement as a function of volume fraction for different activities.

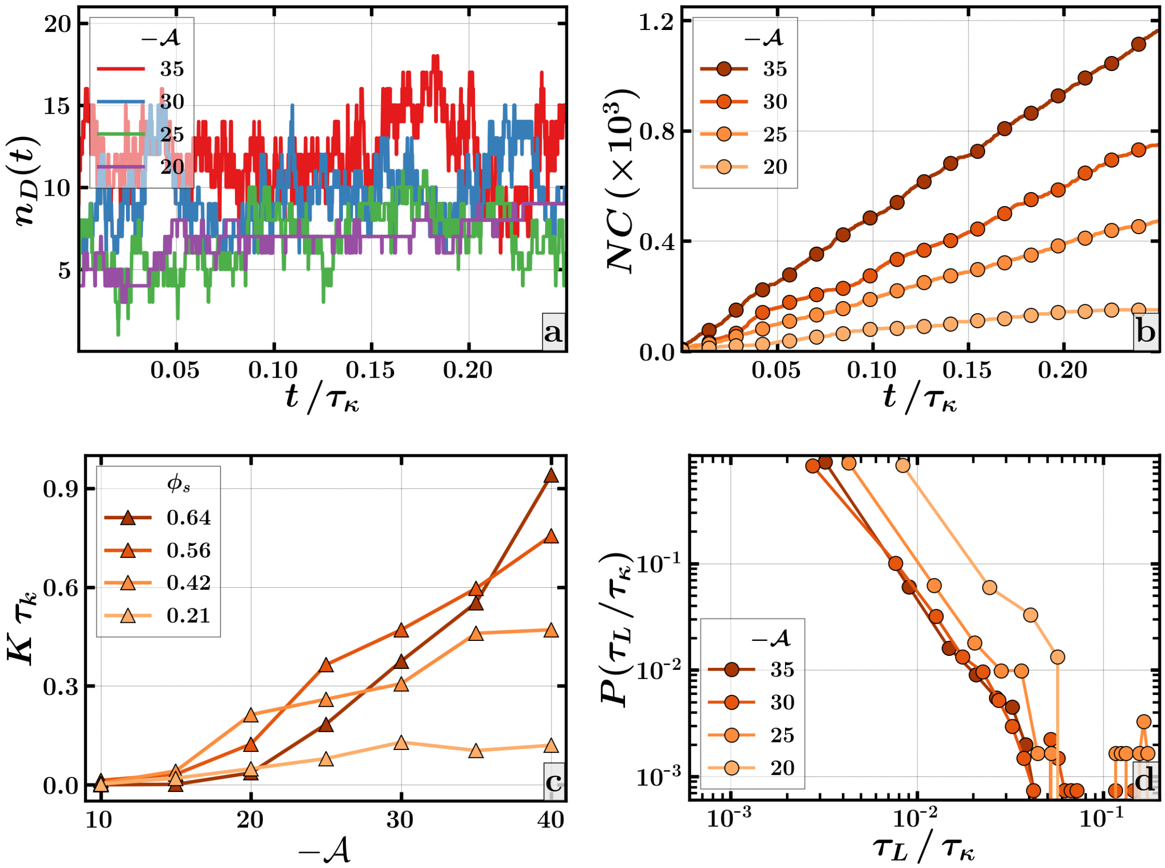


Figure S6. (a) The number of loops and coils in contractile polymers on surface confinement for different acticty. (b) The total number of loops and coils created up to time t, (c) Rate of production of loops and coils for different surface density of the polymer, (d) The life time distribution of the loops and coils.

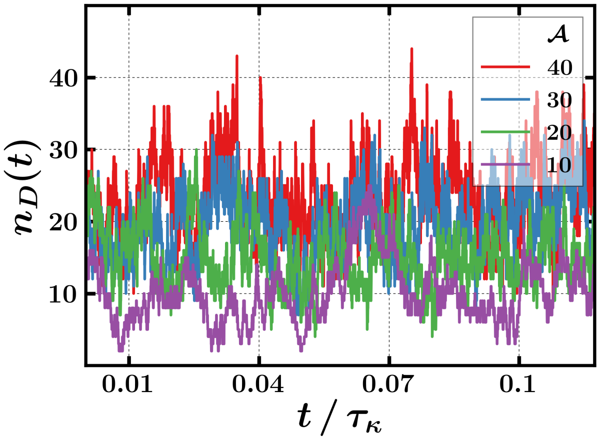


Figure S7. The number of defects, n_D created by extensile active polymers confined on the spherical surface for different values of activity with polymer surface fraction $\phi_s = 0.64$.

IV. DEFECTS DETECTION

Detection of hairpin defects: First we compute local curvature of the polymers at the position of each monomer. The monomer with high curvatures are identified if the curvature is higher that a fixed curvature k_{max}. The monomers with high curvature assigned to a cluster if distance between two monomers are within a distance r_{max}. The cluster of monomers with high curvature is identified as a hairpin defects. We track these hair pin defects and compute the number of polymer associated with it at each time step. The creation and annihilation of defects are determined by the number of monomers in the cluster n_{max}.

Detection of coils and loops: To detect the coils and loops we compute winding number of each polymer on the surface of sphere. Here we approximate that the monomer and its neighbour are in the same plane. We identify polymers with winding number larger than wn_{max}. If center of the these polymers with high winding number are within a distance r_{max}, then they are in the same cluster. We identify these clusters are as loops or coils.

V. SIMULATION PARAMETERS

To solve the equation of motions of active beads, we choose elasticity parameter $k = 5.0$, the equilibrium bond length $b_0 = 2b$ and fluid viscosity $\eta = 1/6$. The length of the active polymer is taken to be $L = 40b_0$. The volume and surface fractions of polymers are varied by changing the number of polymers and keeping radius of confining sphere constant. The strength of the confining potential is chosen as $c = 50$. The dimensionless activity number $\mathcal{A}$ and other parameters used in our simulations are given in the Table S1.

	Contractile	Extensile
Volume confinement	activity number, $\mathcal{A} = [-5, -40]$ bending rigidity, $\kappa = 0.6$ volume fraction, $\phi_v = [0, 0.23]$ confining radius, $R = 15b_0, 25b_0$	activity number, $\mathcal{A} = [5, 40]$ bending rigidity, $\kappa = 0.6$ volume fraction, $\phi_v = [0, 0.23]$ confining radius, $R = 15b_0$
Surface confinement	activity number, $\mathcal{A} = [-5, -180]$ bending rigidity, $\kappa = [0.1, 0.6]$ surface fraction, $\phi_s = [0, 0.68]$ confining radius, $R = 25b_0$	activity number, $\mathcal{A} = [5, 1800]$ bending rigidity, $\kappa = [0.01, 0.6]$ surface fraction, $\phi_s = [0, 0.68]$ confining radius, $R = 25b_0$

Table S1. The list of parameters used in the simulations.

---

[1] Ricca, R. L. & Nipoti, B. Gauss'linking number revisited. *Journal of Knot Theory and Its Ramifications* **20**, 1325–1343 (2011).

[2] Klenin, K. & Langowski, J. Computation of writhe in modeling of supercoiled dna. *Biopolymers* **54**, 307–317 (2000).