Electronic Supplementary Information for *Soft Matter* manuscript: Dynamics of a self-interacting sheet in shear flow

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SI.01: Videos of notable conformational and rotational behaviors

Sheets are hexagonal with circumradius $L = 39a$, where a is the radius of the constitute beads. The beads are in a triangular grid such that each bead has 6 tangent neighbors, totaling $N = 1141$ beads. Sheets were initially in a flat configuration such that all beads lie in the flow-vorticity plane, then rotated by an angle $\theta = 5°$ about the vorticity axis and a variable angle ϕ about the flow axis. Non-neighboring beads were given a hard-sphere potential, while neighbors were given a harmonic potential with spring constant k. Neighboring triangles of three beads (such that they share two beads) were given a dihedral potential with bending rigidity κ. Finally, short-range interactions were applied in the form of a truncated Lennard-Jones potential with interaction strength ε and interaction range $\sigma = 4\sqrt{6}a/3$. All simulations were run at a shear rate of $\dot{\gamma}$ for $\dot{\gamma}t = 2000$ with a time step of $\dot{\gamma}\Delta t = 2 \times 10^{-4}$.

The system was integrated in time using an Euler-Maruyama integrator for Brownian dynamics with hydrodynamics. Please see the main article for details on the potentials, integration scheme, and software.

Simulations are defined by three parameters: χ^{-1}, K, and ϕ. χ^{-1} measures the relative strength of shear to interactions and is given by

$$\chi^{-1} = \frac{6\pi\eta\dot{\gamma}L^2\sigma}{\tilde{\varepsilon}\sigma^2}\left(\frac{L}{a}\right)^{-1}$$

where η is the viscosity, $\tilde{\varepsilon} = \varepsilon/2\sqrt{3}a^2$ is the interaction energy density, and all other parameters are as described earlier. Please see Appendix A of the main article for a derivation of this dimensionless group. K measures the relative strength of bending rigidity to interaction strength and is given by

$$K = \frac{\kappa}{\tilde{\varepsilon}\sigma^2}$$

where κ is the bending rigidity, as described earlier. Finally, ϕ is the initial orientation of the sheet relative to the flow axis, as described earlier.

On the left side of each video is the sheet simulation showing every $0.25\dot{\gamma}t$. All simulation videos were rendered in Ovito[1]. The x-axis is the flow direction, the y-axis is the shear direction, and the z-axis is the vorticity axis. On the right side of each video is the corresponding signed local mean curvature of the sheet. Please see the main article for details on this quantity.

1d_folded_full.mp4 – Example "log-rolling" 1D folded sheet simulation. Simulation parameters are $\chi^{-1} = 4.1 \times 10^1$, $K = 0.03$, $\phi = 0°$.

2d_folded_full.mp4 – Example 2D folded sheet simulation. Simulation parameters are $\chi^{-1} = 1.4 \times 10^0$, $K = 0.03$, $\phi = 0°$.

flat_full.mp4 – Example flat sheet simulation. Simulation parameters are $\chi^{-1} = 1.4 \times 10^2$, $K = 10.0$, $\phi = 0°$.

low_vdotz_full.mp4 – Example 1D folded sheet with largest axis rotating about the vorticity axis. Simulation parameters are $\chi^{-1} = 4.1 \times 10^1$, $K = 0.003$, $\phi = 45°$.

rolled_up.mp4 – Example rolled-up sheet simulation. Simulation parameters are $\chi^{-1} = 1.4 \times 10^2$, $K = 0.03$, $\phi = 0°$.

teacup_full.mp4 – Example sheet simulation exhibiting teacup behavior. Simulation parameters are $\chi^{-1} = 4.1 \times 10^2$, $K = 0.003$, $\phi = 85°$.

tumbling_full.mp4 – Example tumbling sheet simulation. Simulation parameters are $\chi^{-1} = 1.4 \times 10^3$, $K = 0.03$, $\phi = 0°$.

SI.02: Gyration tensor eigenvalue histograms

The ij'th component of the gyration tensor, $\boldsymbol{S}$, is given by

$$S_{ij} = \frac{1}{N}\sum_{k=1}^{N}\left(r_i^{(k)} - \bar{r}_i\right)\left(r_j^{(k)} - \bar{r}_j\right)$$

where N is the number of particles in the sheet, $r_i^{(k)}$ is the i'th component of the position of particle k, and $\bar{r}_i$ is the i'th component of the center of mass of the particles. The square root of the eigenvalues of $\boldsymbol{S}$, λ_i, give a measure of the characteristic sizes of the sheet, while their standard deviation gives a measure of how much these sizes fluctuate, and thus how much the sheet deforms over time. We can use these values to distinguish between different sheet conformations. Please see the main article for details on the criteria used.

For a given simulation snapshot, we define $\lambda_1 > \lambda_2 > \lambda_3$. For each simulation, we define $\bar{\lambda}_i$ to be the average of λ_i and std[λ_i] to be the standard deviation of λ_i, both over the last $250\dot{\gamma}t$ such that start-up effects are not included.

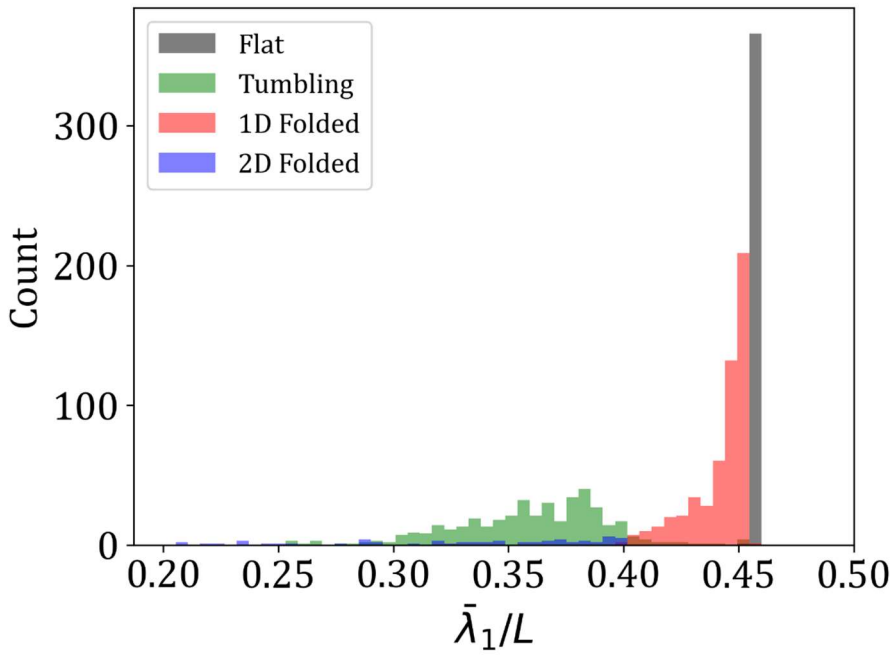

Figure S02.01: Histogram of the average square root of the largest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

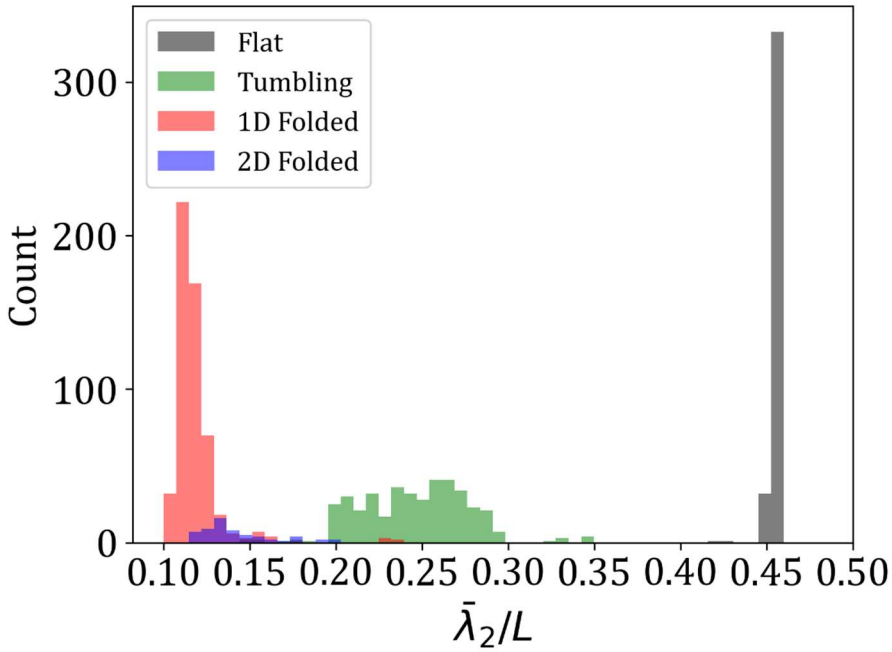

Figure S02.02: Histogram of the average square root of the second largest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

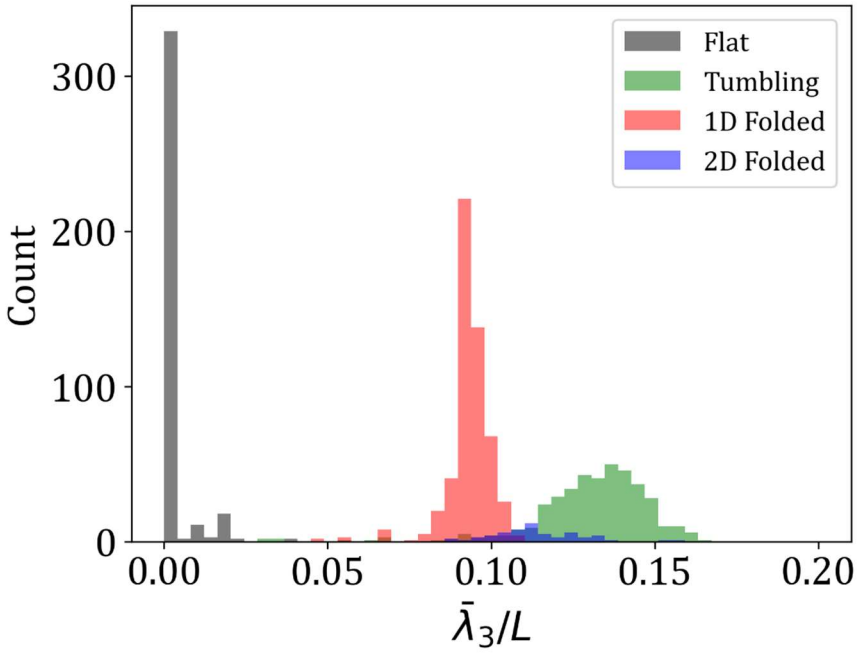

Figure S02.03: Histogram of the average square root of the smallest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

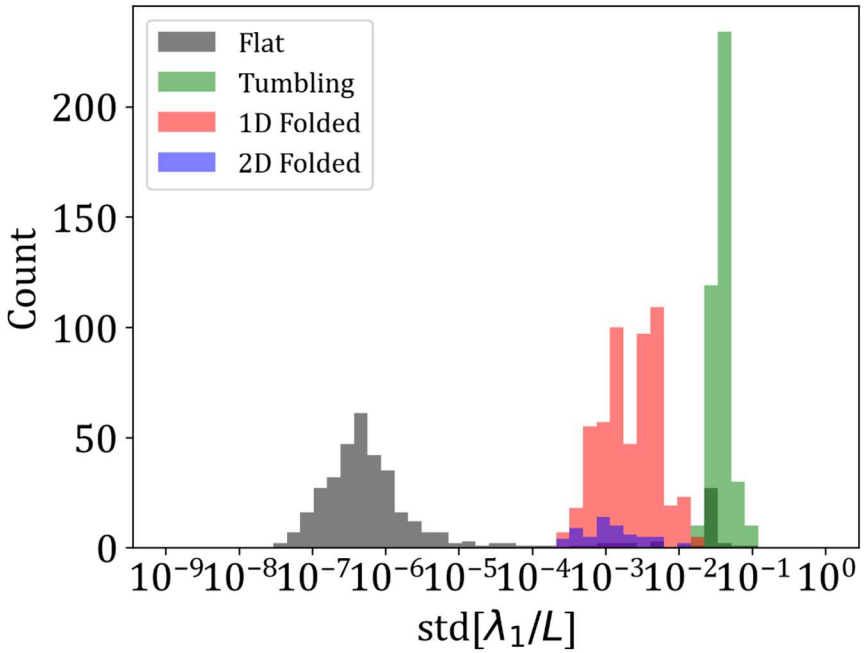

Figure S02.04: Histogram of the standard deviation of the square root of the largest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

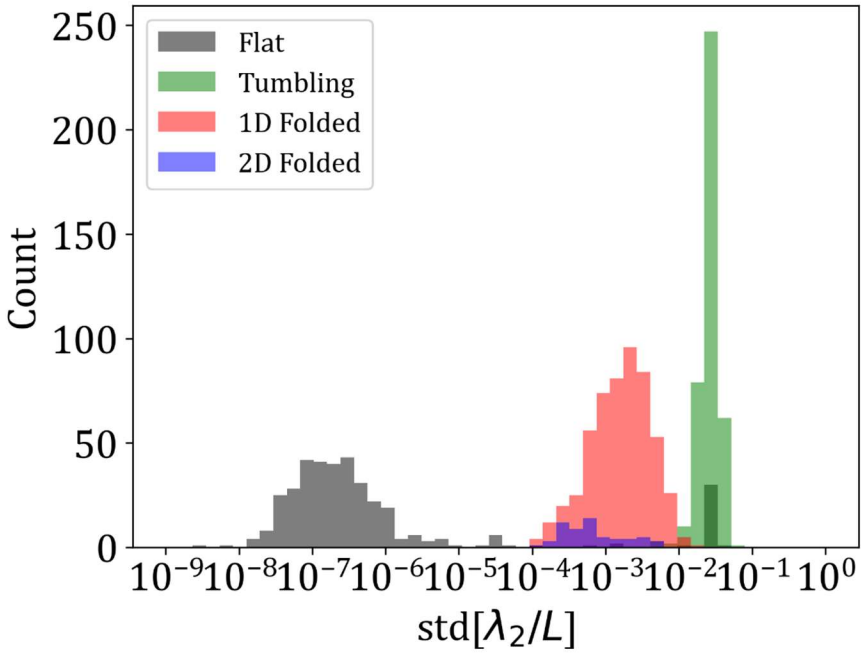

Figure S02.04: Histogram of the standard deviation of the square root of the second largest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

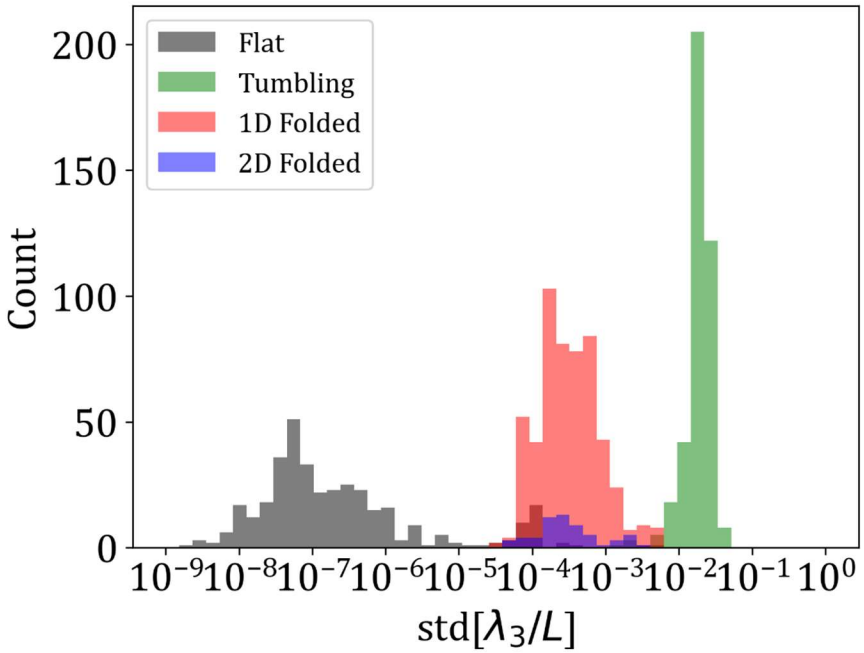

Figure S02.05: Histogram of the standard deviation of the square root of the smallest eigenvalue of the gyration tensor over the last $200\dot{\gamma}t$ of each simulation.

SI.03: Scatter plots of sheet viscosity versus sheet summary statistics

The radius of gyration is given by the square root of the sum of the eigenvalues of the gyration tensor:

$$R_g = \sqrt{\sum \lambda_i^2}$$

The radius of gyration is a measure of the overall **size** of a sheet. The relative shape anisotropy can similarly be defined in terms of the eigenvalues of the gyration tensor:

$$\zeta^2 = \frac{3}{2}\frac{\sum \lambda_i^4}{(\sum \lambda_i^2)^2} - \frac{1}{2}$$

The relative shape anisotropy is bounded between 0 and 1. $\zeta^2 = 0$ only if the beads are spherically symmetric and $\zeta^2 = 1$ only if the beads are all colinear. The relative shape anisotropy is therefore a measure of the **shape** of a sheet.

The alignment is given by the magnitude of the dot product of the unit vector pointing in the same direction as the largest axis of the minimum bounding ellipsoid, $\boldsymbol{v}_1$, with the vorticity axis, $\hat{z}$: $|\boldsymbol{v}_1 \cdot \hat{z}|$. The alignment is therefore a measure of the **orientation** of a sheet.

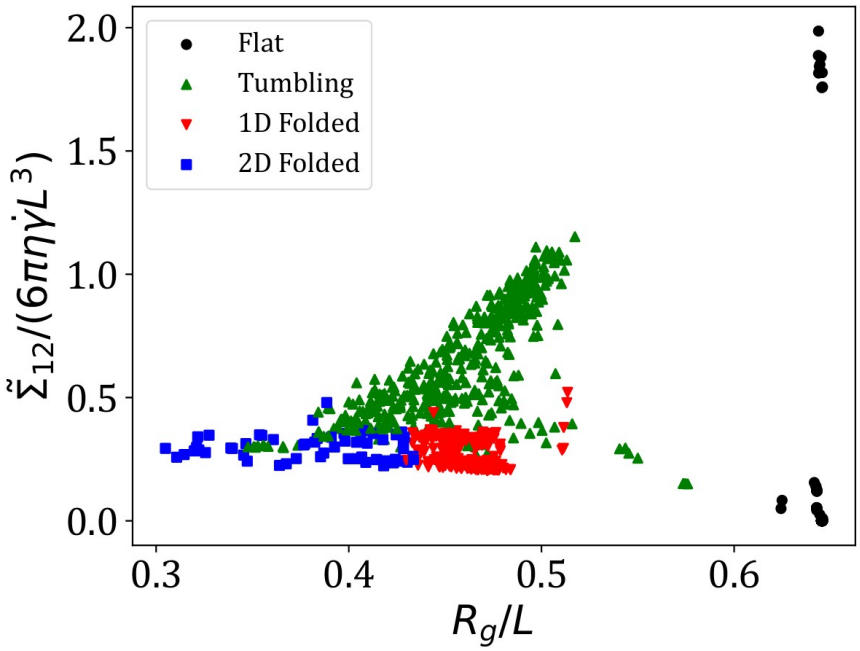

Figure S03.01: Scatter plot of the sheet viscosity as a function of the average radius of gyration over the last $200\dot{\gamma}t$ of each simulation. Points are colored based on their conformational identity.

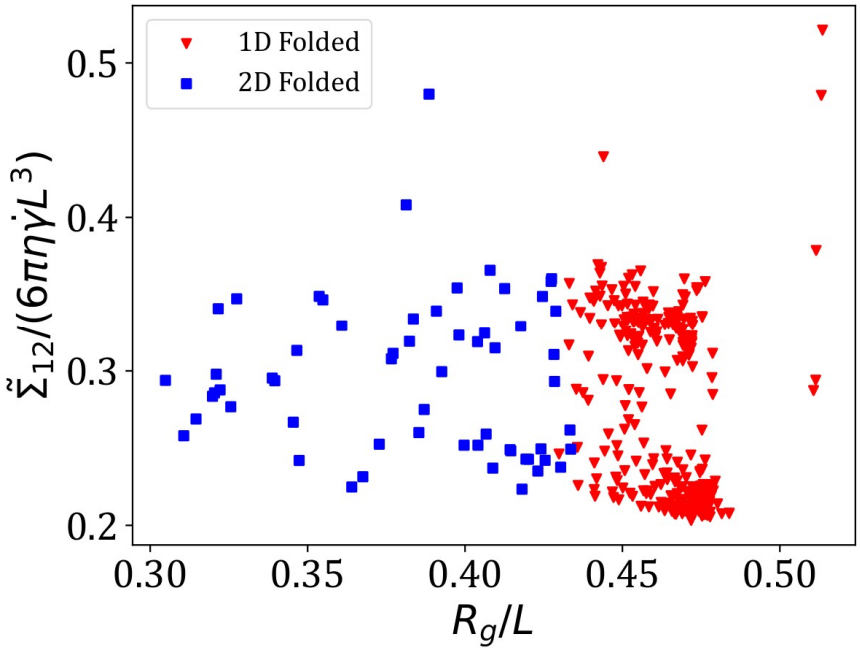

Figure S03.02: Scatter plot of the sheet viscosity as a function of the average radius of gyration over the last $200\dot{\gamma}t$ of each simulation for only folded sheets. Points are colored based on their conformational identity.

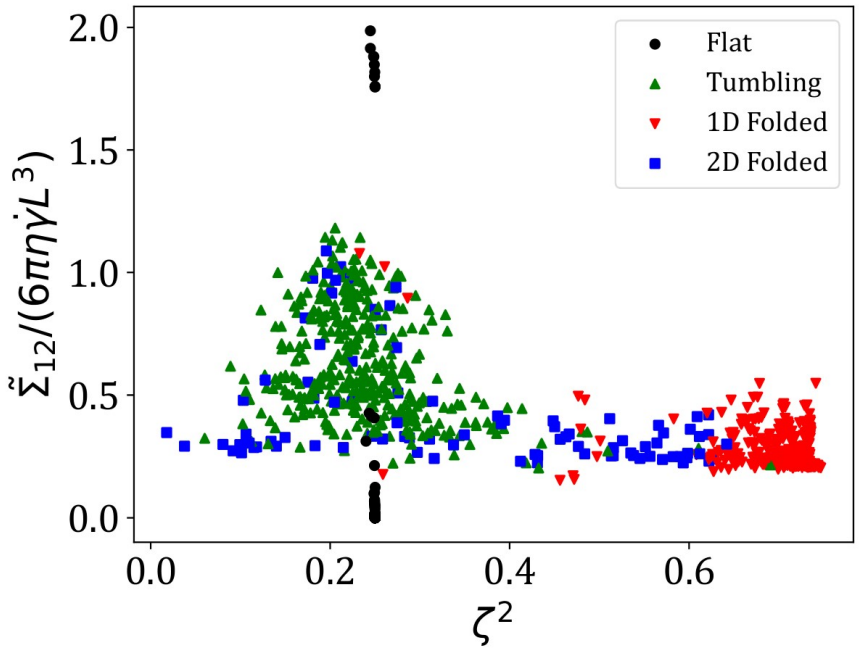

Figure S03.03: Scatter plot of the sheet viscosity as a function of the average relative shape anisotropy over the last $200\dot{\gamma}t$ of each simulation. Points are colored based on their conformational identity.

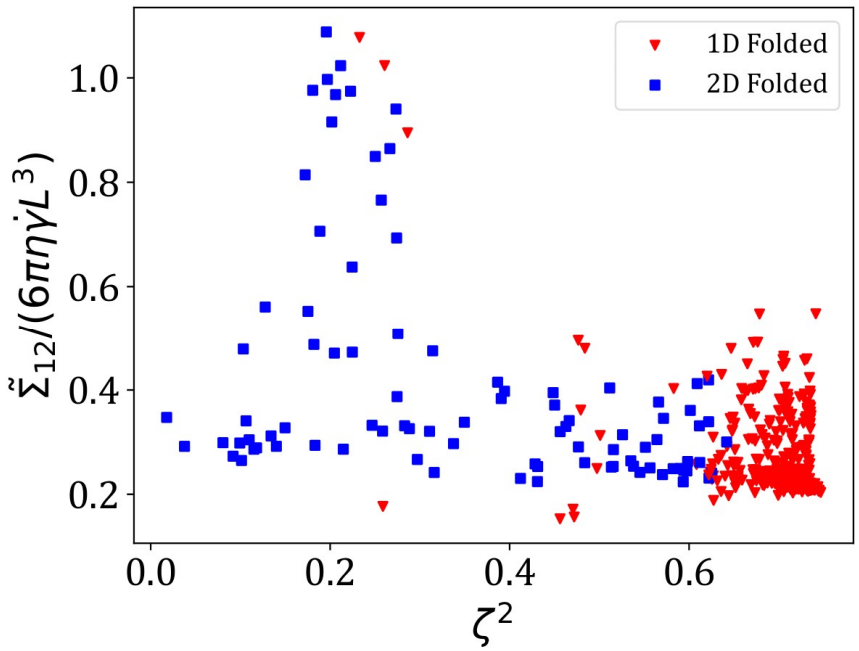

Figure S03.04: Scatter plot of the sheet viscosity as a function of the average relative shape anisotropy over the last $200\dot{\gamma}t$ of each simulation for only folded sheets. Points are colored based on their conformational identity.

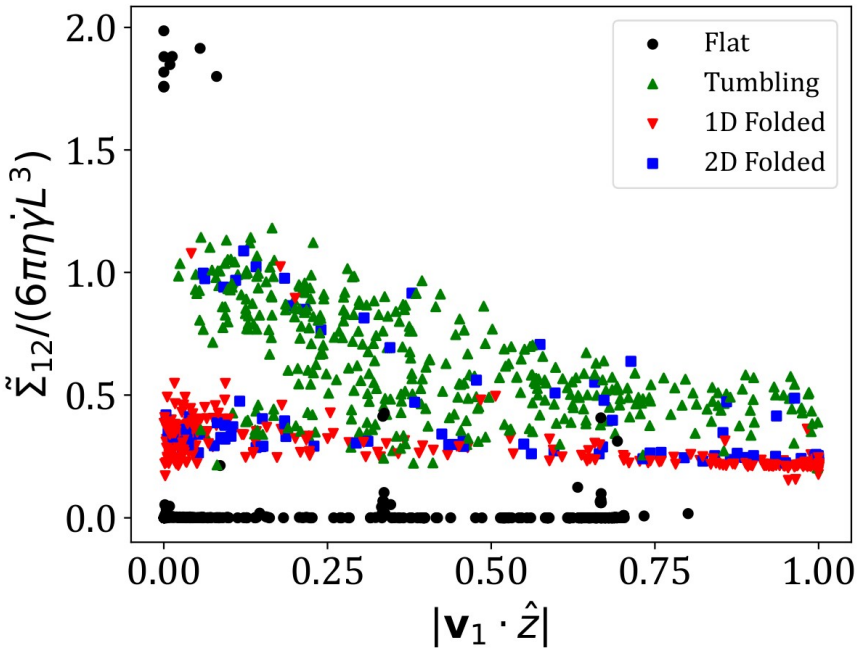

Figure S03.05: Scatter plot of the sheet viscosity as a function of the average alignment over the last $200\dot{\gamma}t$ of each simulation. Points are colored based on their conformational identity.

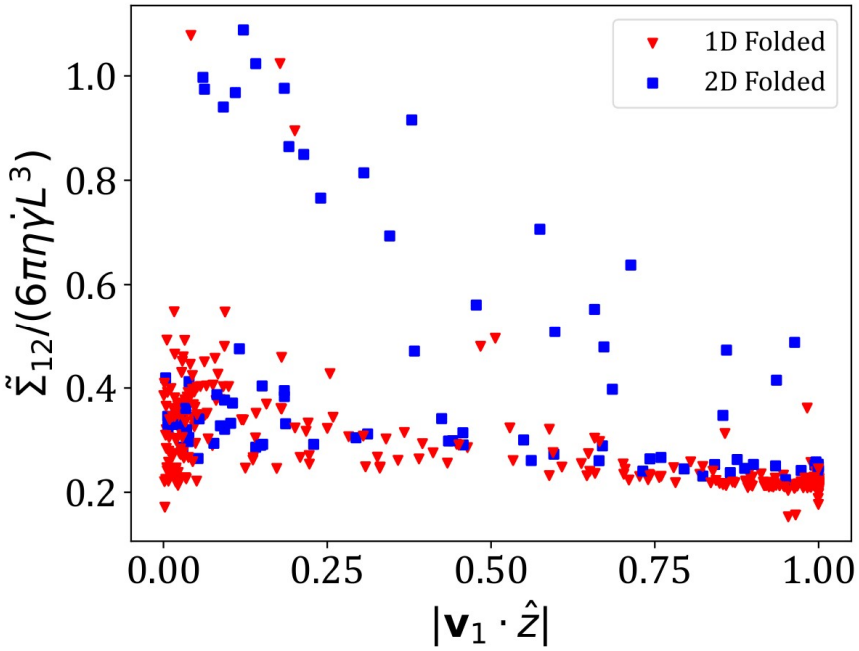

Figure S03.06: Scatter plot of the sheet viscosity as a function of the average alignment over the last $200\dot{\gamma}t$ of each simulation for only folded sheets. Points are colored based on their conformational identity.

SI.04: References

[1]Stukowski, A. (2009). Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and simulation in materials science and engineering*, *18*(1), 015012.