Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information for: Ruptures of Mixed Lipid Monolayers Under Tension and Supercooling: Implications for Nanobubbles in Plants

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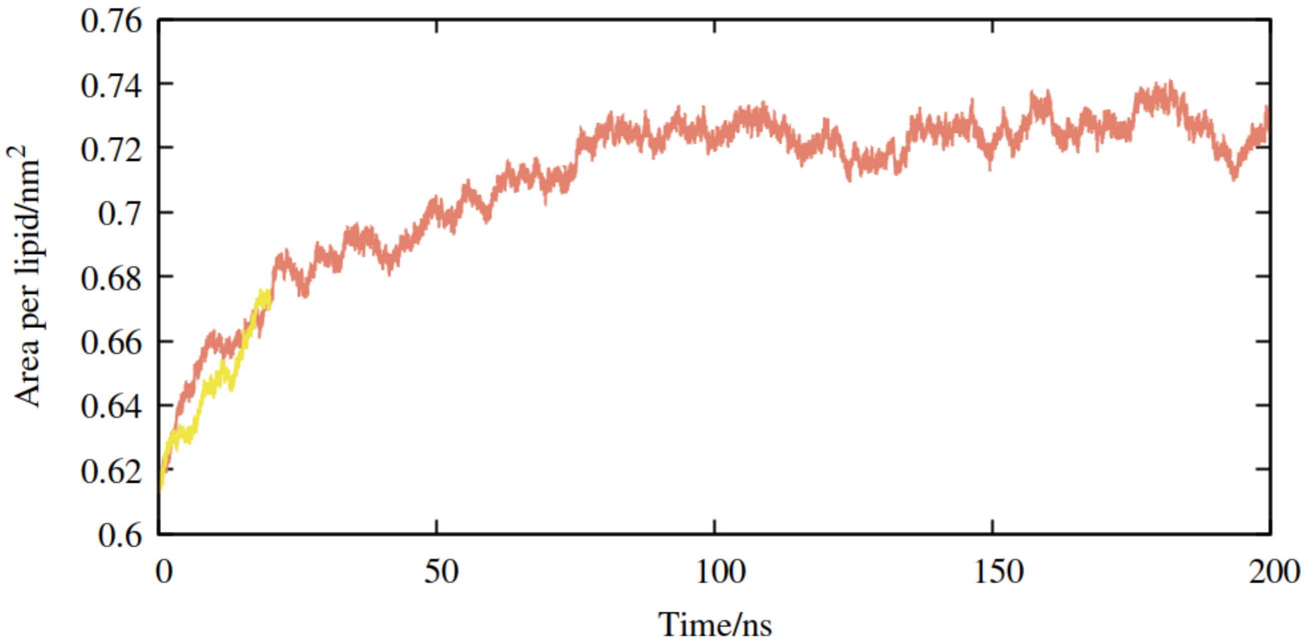

Figure S1: Expansion of the mixed monolayer at $T = 270$ K and $p = -2.5$ MPa. Two simulations are presented, with the same starting coordinates, but differing random seeds for velocity generation. Yellow data is the same as that presented in the second trajectory of Figure 3 in the main text.

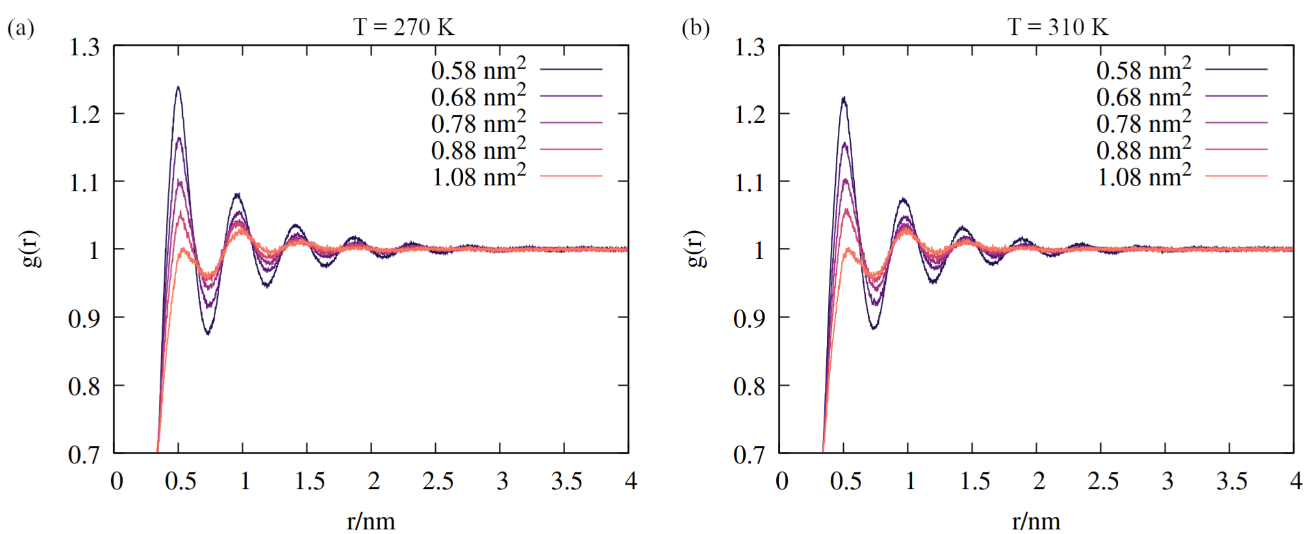

Figure S2: Two dimensional radial distribution functions (RDFs) of lipid tail group atoms, at increasing areas per lipid. (a) $T = 270$ K and (b) $T = 270$ K. RDFs were calculated using the same atomic coordinates as those presented in Figure 4 in the main text, output every 10 ps between $t = 10$ and 60 ns.

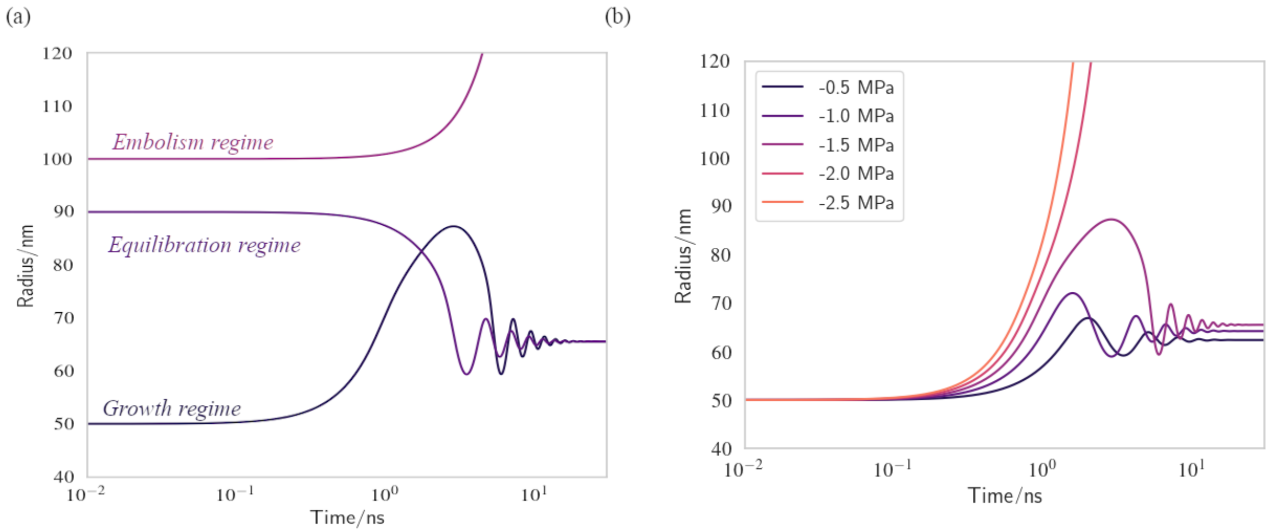

Figure S3: Bubble dynamics produced by integration of the Rayleigh-Plesset equation (Eq. 7), assuming $T = 310$ K, $N_{\text{lipids}} = 10^5$, and a dynamic surface tension $\gamma(r)$. (a) $p = -1.5$ MPa, with varying starting radii, r_0. (b) r_0=50 nm, with varying external negative pressure, p. Further details in main text and Methods.

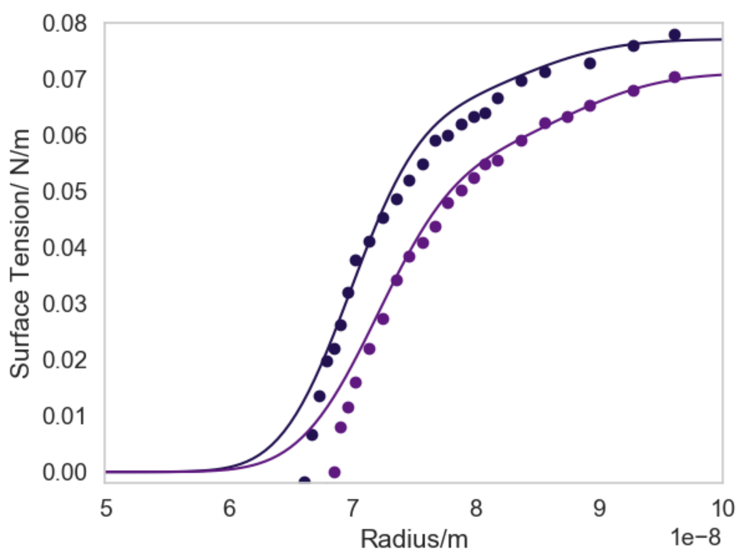

Figure S4: Smoothed parameterisations of the calculated surface tensions, $\gamma_{\text{MD}}(T)$, as a function of radius, r, where $r = \sqrt{(APL \cdot N_{\text{Lipids}})/4\pi}$. Purple points and lines are at $T = 310$ K, black are at $T = 270$ K.