

Calculations:1) Estimate of $H(Q_{II}^D)$ and $H(Q_{II}^G)$

In order to determine a surface-averaged mean curvature for a monolayer, we must first define a specific surface within the monolayer, since the curvature at the headgroup region is different to that at the tips of the hydrophobic chains. Following the approach described by Templer et al¹, we use the “pivotal surface” – the surface where the area per molecule does not change on monolayer bending – which we consider to lie parallel to the underlying minimal surface. In order to determine its position, we solve the equation $\phi_w = 1 - \frac{v}{v_n} \left(2\sigma_0 \frac{\xi}{a} + \frac{4}{3} \pi \chi \left(\frac{\xi}{a} \right)^3 \right)$ to find its distance ξ from the minimal surface. χ and σ_0 are respectively the Euler characteristic and the dimensionless minimal surface area per unit cell. These take values of $\chi = -2$ and $\sigma_0 = 1.919$ for the D minimal surface, and $\chi = -8$ and $\sigma_0 = 3.091$ for the G. v and v_n are the total molecular volume and the molecular volume on the hydrophobic side of the pivotal surface; we use values of $v = 0.612 \text{ nm}^3$, $v_n = 0.465 \text{ nm}^3$ for 1-monolein, taken from Templer et al². ϕ_w and a are the water volume fraction and lattice parameter, respectively. The data we analyse here are taken from a sample with $\phi_w = 0.32$, where the Q_{II}^D and Q_{II}^G phases being inter-converted have lattice parameters $a = 8 \text{ nm}$ and $a = 13.2 \text{ nm}$ respectively³. From these data we calculated the distance of the pivotal surface from the minimal surface to be $\xi = 1.125 \text{ nm}$ for Q_{II}^D and $\xi = 1.151 \text{ nm}$ for Q_{II}^G .

We also require the average Gaussian curvature for the underlying minimal surface in each structure. This is given by¹ $\langle K \rangle = \frac{2\pi\chi}{\sigma_0 a^2}$ and has values of -0.103 nm^{-2} and -0.094 nm^{-2} for the Q_{II}^D and Q_{II}^G phases respectively, with the lattice parameters in this experiment.

The mean curvature for a pivotal surface lying a distance ξ from a minimal surface of Gaussian curvature K is given by² $H_n = \frac{K\xi}{1 + K\xi^2}$. From the values calculated above, we obtain the values of $H(Q_{II}^D) = -0.133 \text{ nm}^{-1}$ and $H(Q_{II}^G) = -0.123 \text{ nm}^{-1}$. (For simplicity we have omitted the brackets denoting surface averaging, and the subscript n, in the body of the text.)

2) Estimate of the number of molecules per unit cell

In our estimate of the number of unit cells corresponding to a certain number of molecules (specifically, the cooperative unit) we estimate the area of monolayer pivotal surface within one unit cell by noting that the area of a parallel (eg pivotal) surface projected a distance z from a minimal surface of Gaussian curvature K and area $A(0)$ is given by² $A(z) = A(0)(1 + Kz^2)$. There are two monolayers within the unit cell, the area of the minimal surface within the unit cell is given by $A(0) = \sigma_0 a^2$, and each lipid molecule has an area at the pivotal surface given by A_n . The total number of molecules within one unit cell is therefore $\frac{2\sigma_0 a^2 (1 + \langle K \rangle \xi^2)}{A_n}$.

Using lattice parameter values as above, and the value for area per lipid molecule for 1-monoolein of $A_n = 0.33 \text{ nm}^2$ (from Templer et al²), we estimate that a unit cell of the Q_{II}^D phase contains 650 molecules, while one of the Q_{II}^G phase contains 2860.

1. R. H. Templer, J. M. Seddon, N. A. Warrender, A. Strykh, Z. Huang, R. Winter and J. Erbes, *J. Phys. Chem. B*, 1998, **102**, 7251-7261.

Supplementary Material (ESI) for Soft Matter

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2. R. H. Templer, B. J. Khoo and J. M. Seddon, *Langmuir*, 1998, **14**, 7427-7434.