Molecular structure of the lecithin ripple phase

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Supporting Information

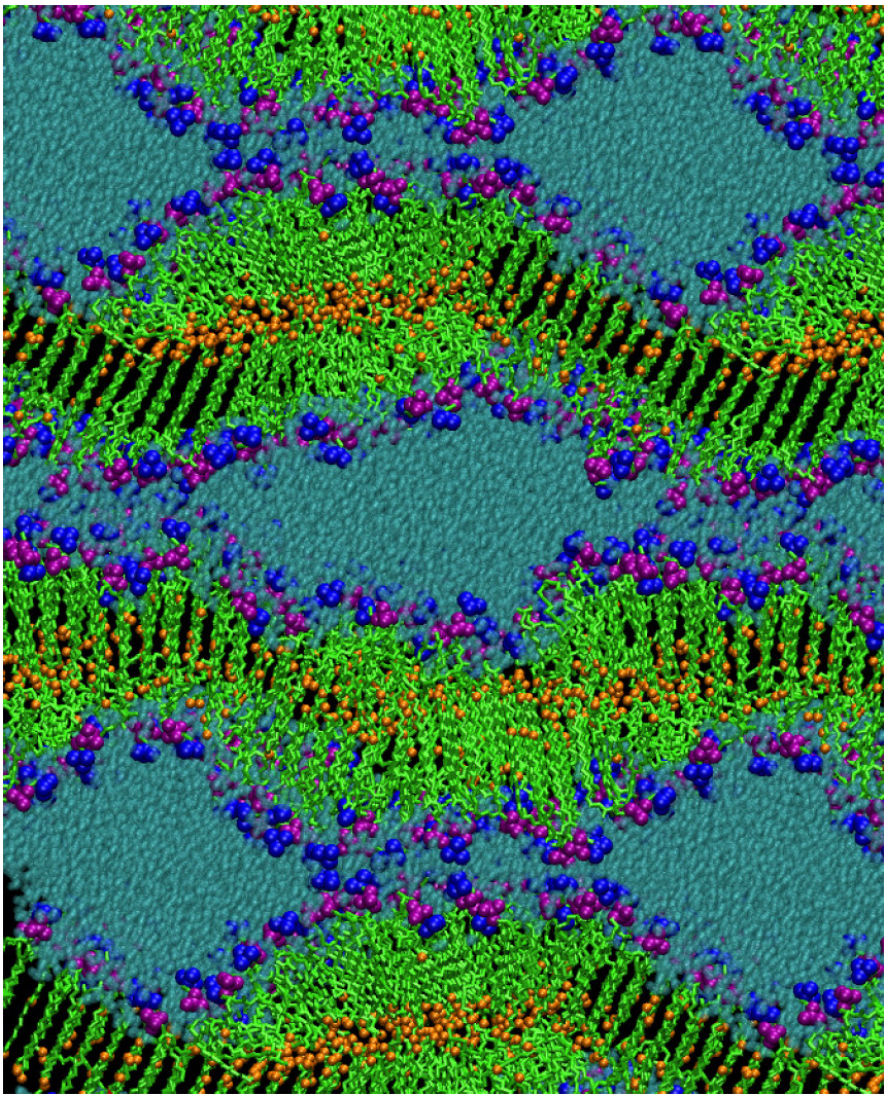

Fig. 5. Snapshot of an intermediate ripple structure for DPPC in water. The color scheme is the same as used in Fig. 2. The snapshot was taken after 250 ns of simulation at 283 K of a system containing 392 lipids and 23 water molecules per lipid, starting from a Lα structure. The simulation box contains two independent lipid bilayers, containing 196 lipids each. Parts of the periodic images of the independent bilayers are shown. Note that the ordering of the acyl chains has reached different stages in both bilayers, but that the overall ripple structure characteristics are similar to those shown in Fig. 2.

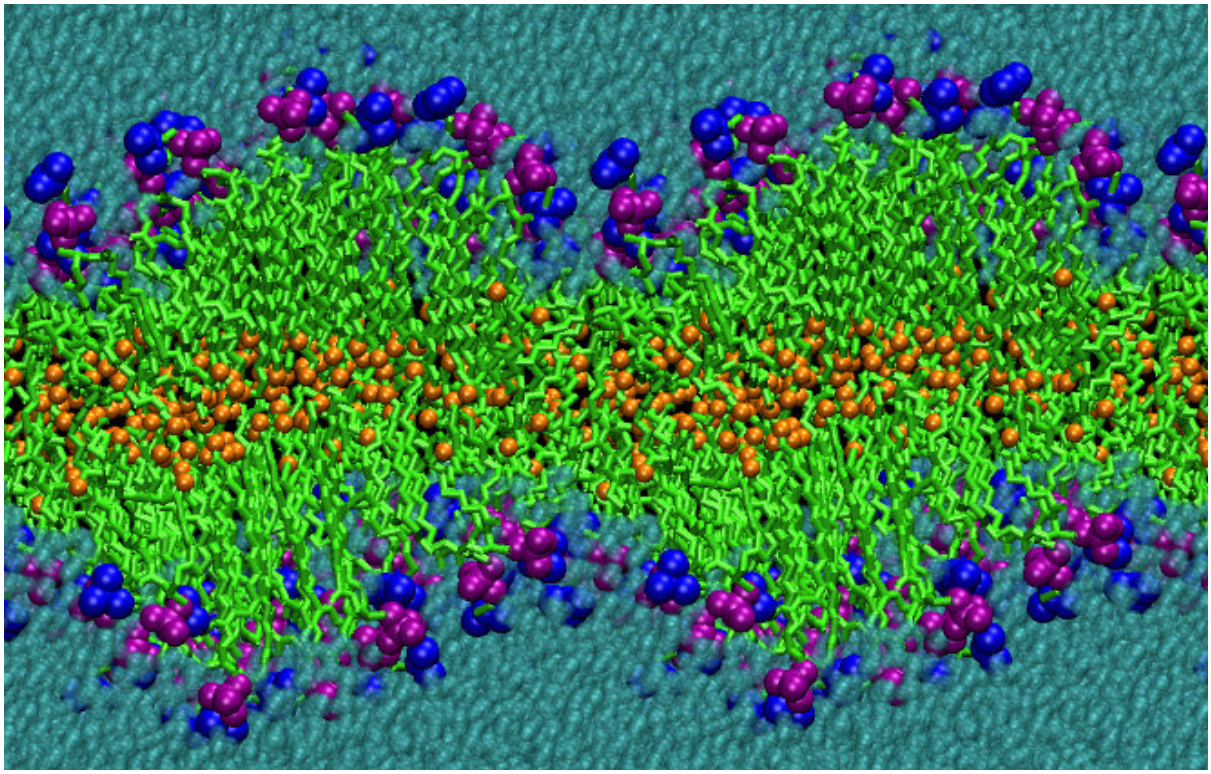

Fig. 6. Snapshot of a peristaltic ripple structure for DPPC in water. The color scheme is the same as that of Fig. 2. The snapshot was taken after 54 ns of simulation at 283 K of a system containing 64 lipids and 23 water molecules per lipid, starting from an Lα structure. Two replicas of the simulation box are shown. These structures are formed because there are not enough lipids available to form a *m* domain and two kink regions between two periodic copies of a gel-like domain (there is one gel-like domain in the periodic box). This peristaltic structure is similar to the one found by Kranenburg *et al*. (1) using dissipative particle dynamics simulations of a coarse-grained model.

1. Kranenburg, M, Laforge, C. & Smit, B. (2004) *Phys. Chem. Chem. Phys.* **6**, 4531-4534.

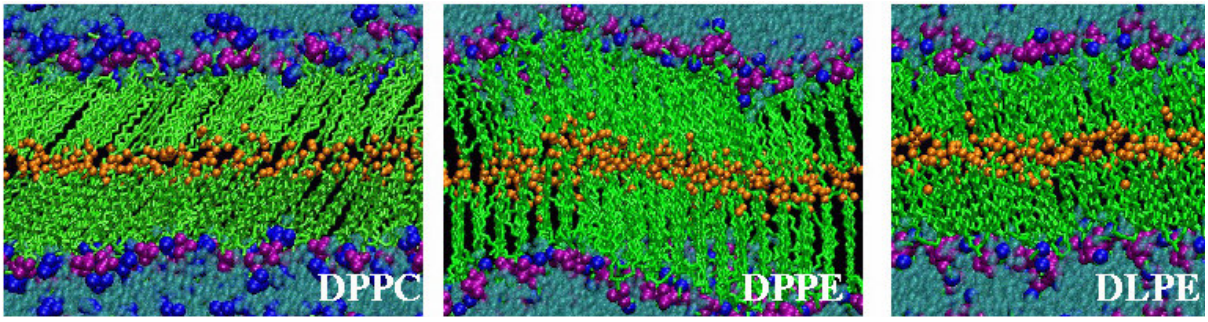

Fig. 7. Snapshots of gel structures of DPPC, dipalmitoylphosphatidylethanolamine (DPPE), and dilauroylphosphatidylethanolamine (DLPE) in water. The color scheme is the same as used in Fig. 2. The gel structures are characterized by the high degree of ordering of the lipid tails, which contain only a few gauche defects. All structures formed spontaneously, starting from a Lα structure. (*Left*) DPPC. The snapshot was taken after 300 ns of simulation at 283 K of a system containing 196 lipids and 10 water molecules per lipid. Note the uniform tilt of the acyl chains. (*Middle*) DPPE. The snapshot was taken after 140 ns of simulation at 303 K of a system containing 256 lipids and 23 water molecules per lipid. The lipids are less tilted than in the DPPC structure. An undulation of the bilayer is visible. This undulation is suppressed at lower hydration. (*Right*) DLPE. The snapshot was taken after 300 ns of simulation at 283 K of a system containing 64 lipids and 10 water molecules per lipid. The acyl chains are less well packed than in the gels of DPPC and DPPE.

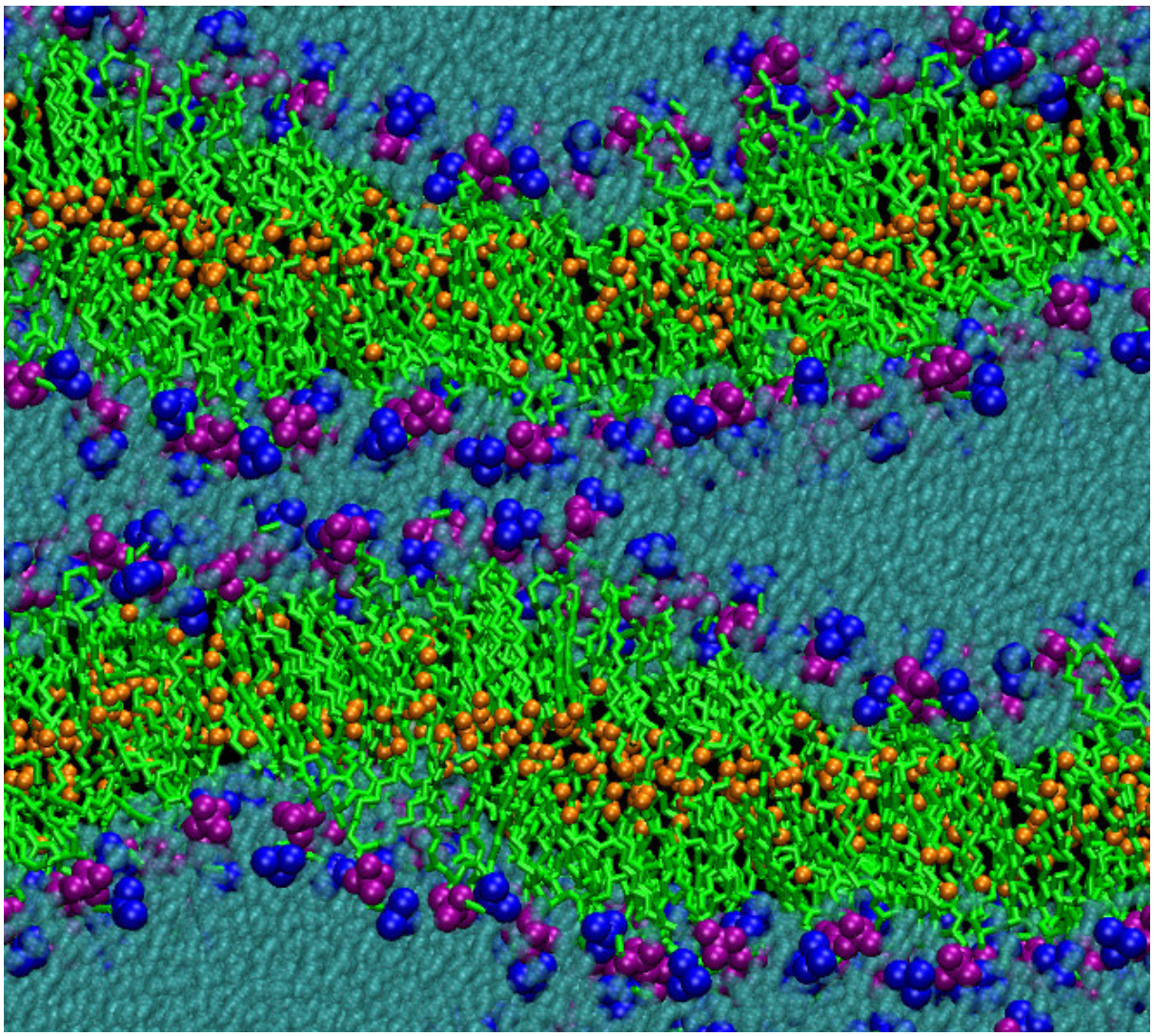

Fig. 8. Snapshot of a ripple structure for dilauroylphosphatidylcholine (DLPC) in water. The color scheme is the same as used in Fig. 2. This structure was formed after 40 ns of simulation at 258 K of a system containing 256 lipids and 21 water molecules per lipid, starting from a Lα structure. Two replicas of the simulation box are shown. The overall ripple structure is clearly visible, but ordering of the lipid tails is less strong than for DPPC. Interdigitation is seen in the *m* domain. DLPC ripple characteristics are: λ_r, 18 nm; d, 5.5 nm; γ, 128°; x_0, 13 nm; A, 3.0 nm; d_M, 3.4 nm; w_M, 1.5 nm; d_m, 2.9 nm; and w_m, 4.5 nm.