Supporting Information:

Coarse-grained molecular dynamics simulation of cation distribution profiles on negatively charged lipid membranes during phase separation

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Hydration state of sodium ion

The all-atomic molecular dynamics (MD) simulation of Na^+ and Cl^- ions solution consisting of 602 atoms in total is performed for 120 ps under three-dimensional periodic boundary conditions. An ion concentration is set at 217 mM. The third-order density-functional tight-binding (DFTB3) method is used with DFTB+[S1] (version 20.1) open-source software. Parameter sets of 3ob[S2,S3] and 3obw[S4] are used with H5 correction.[S5] The temperature is kept constant at 300 K by a Nose-Hoover thermostat[S6] with a coupling strength of 3200 cm^{-1}. A pressure of 1 atm was controlled isotropically by a Berendsen barostat[S7] with a damping time of 0.1 ps. The velocity-Verlet algorithm with a time step of 1 fs is used for the integration of the equations of motion.
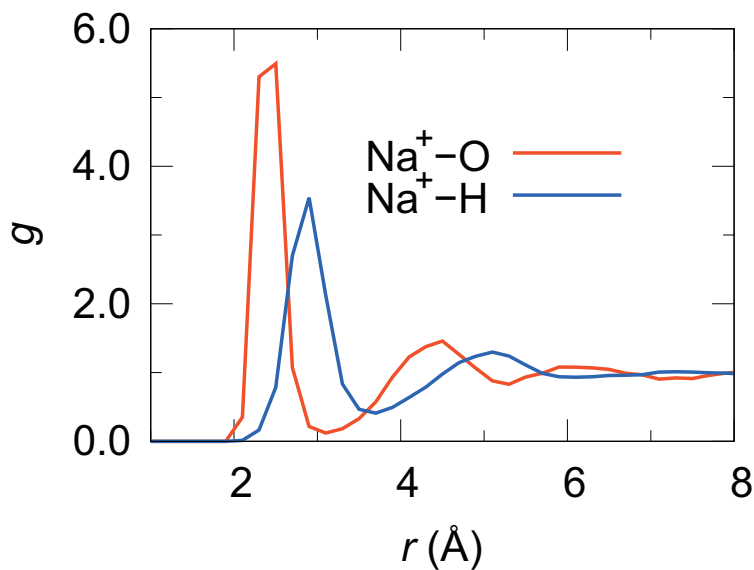

Figure S1: Radial distribution functions (RDFs), $g(r)$, of water molecules around a sodium ion by the all-atomic molecular dynamics (MD) simulation based on a third-order density functional tight-binding (DFTB3) method.
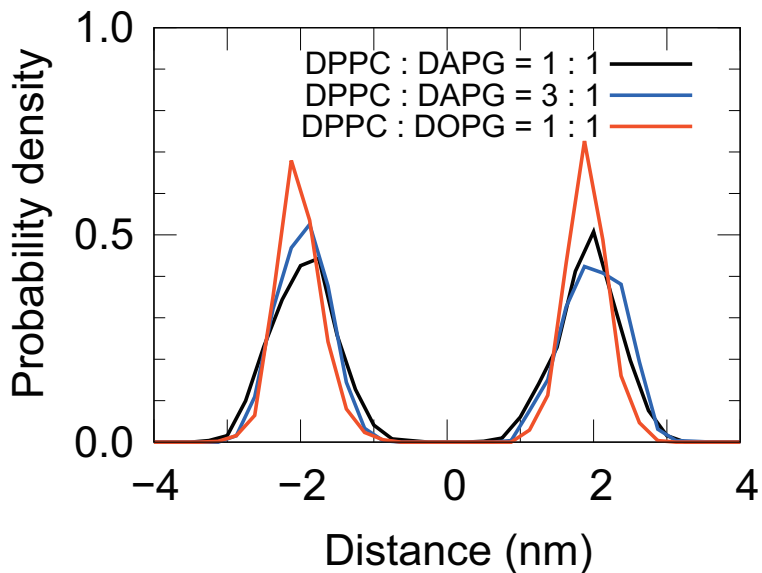
Surface roughness

Figure S2: The probability density of the negatively charged PO_4^- group along z-direction (perpendicular to the membrane surface) at 5 µs for DPPC:DAPG = 1 : 1 mixture, DPPC:DAPG = 3 : 1, and DPPC:DAPG = 1 : 1 with a NaCl concentration of 100 mM.

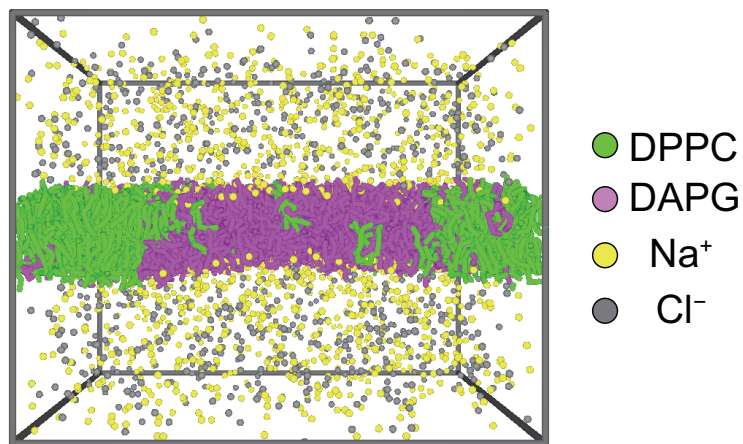Figure S3: The snapshot of the side view of the membrane at 5 µs for DPPC:DAPG = 1 : 1 mixture with a NaCl concentration of 100 mM.

References

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