

[Supporting Information]

Formation of Nanopores in DiynePC-DPPC Complex Lipid Bilayers Triggered by On-Demand Photo-Polymerization

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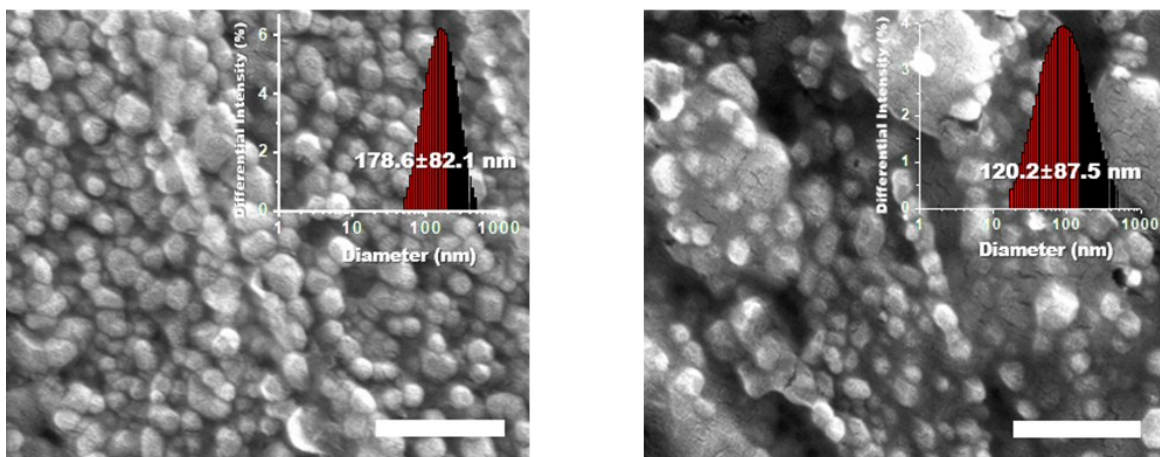


Figure S1. SEM images of DPPC/DiynePC vesicles (left) and DOPC/DiynePC vesicles (right); scale bar: 500 nm. (Insets show size distributions of both samples)

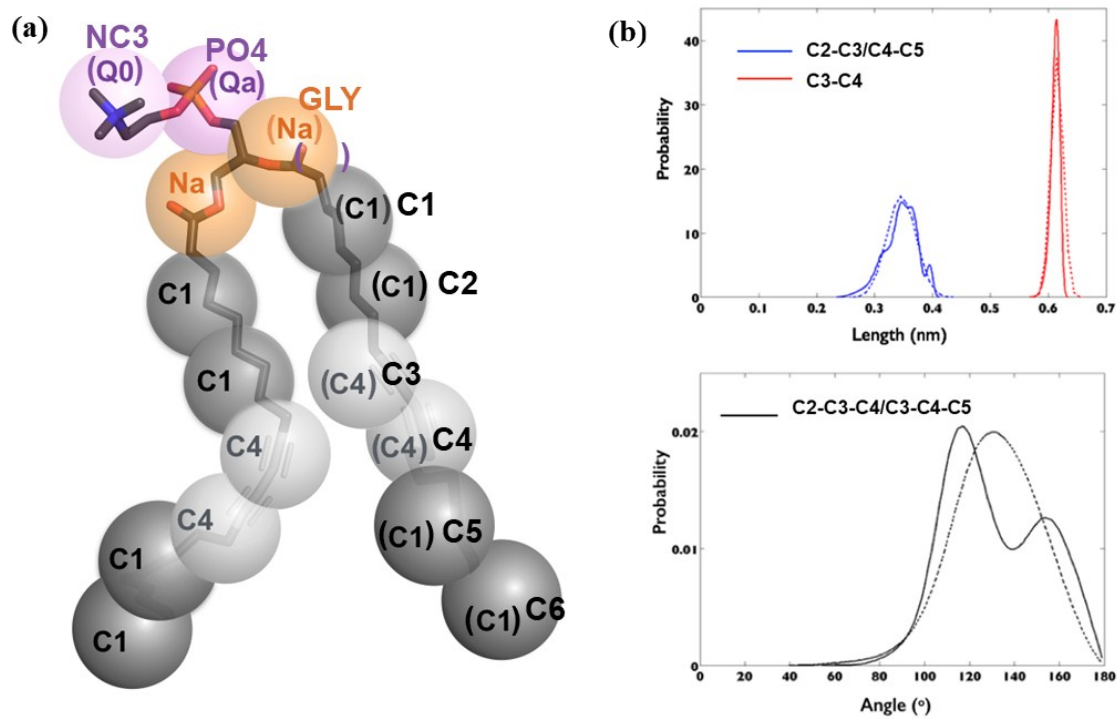


Figure S2. (a) CG mapping scheme (b) bond and angle distributions of DiynePC. Solid line and dotted line obtained from AA and CG simulation, respectively.

Table S1. Martini FF parameters for DiynePC

Bond	Func. type	r_0(nm)	K_b(kJ/mol nm²)
C1-C4	1	0.36	6000
C4-C4	1	0.61	Const.
Angle	Func. type	θ_0(deg)	K_θ(kJ/mol)
C4-C4-C1	1	140	20
C4-C1-C1	2	180	25

Table S2. Overview of the CG simulation setup.

Matrix lipid	Molar ratio of matrix/DiynePC	no. of matrix lipid	no. of DiynePC	no. of water^a	Simulation time (μs)
DPPC	2:1	2700	1350	30375	5
DOPC	2:1	2700	1350	30375	5

^aNumber of CG water particles. The corresponding number of real water molecules is 4 times higher.

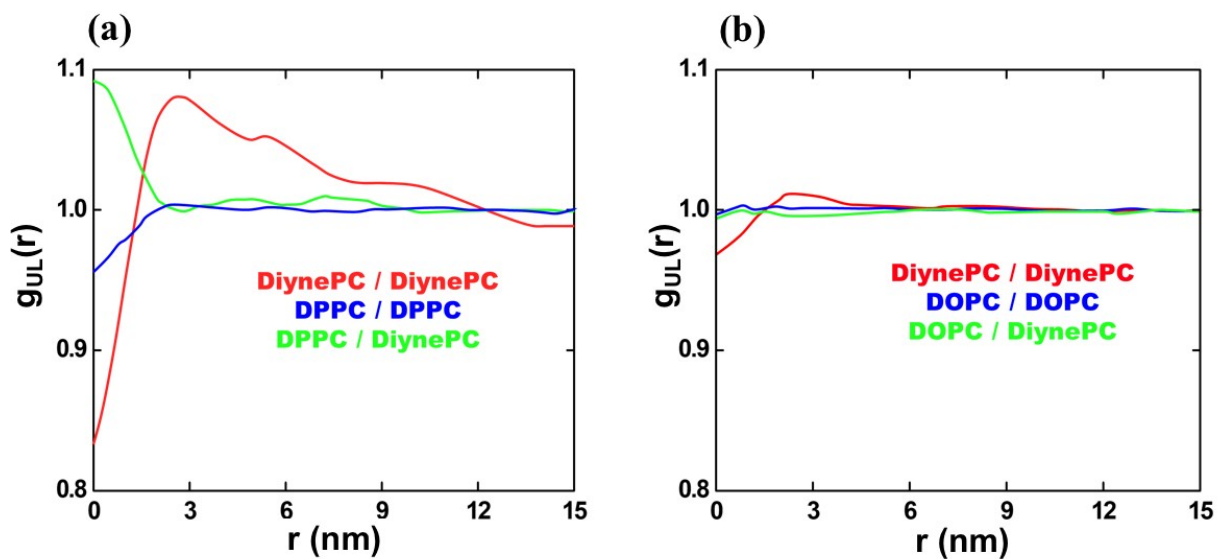


Figure S3. Radial distribution functions (RDFs) of glycerol centers of the lipids for the (a) DPPC/DiynePC (2:1) mixture and (b) DOPC/DiynePC (2:1) mixture; probability of occurrence of pair forms in DiynePC/DiynePC, matrix lipid/matrix lipid, and matrix lipid/DiynePC drawn compared to random mixing having RDF of 1. Radial distribution functions of glycerol centers of the lipids with different leaflets of the bilayer for the (c) DPPC/DiynePC and (d) DOPC/DiynePC.

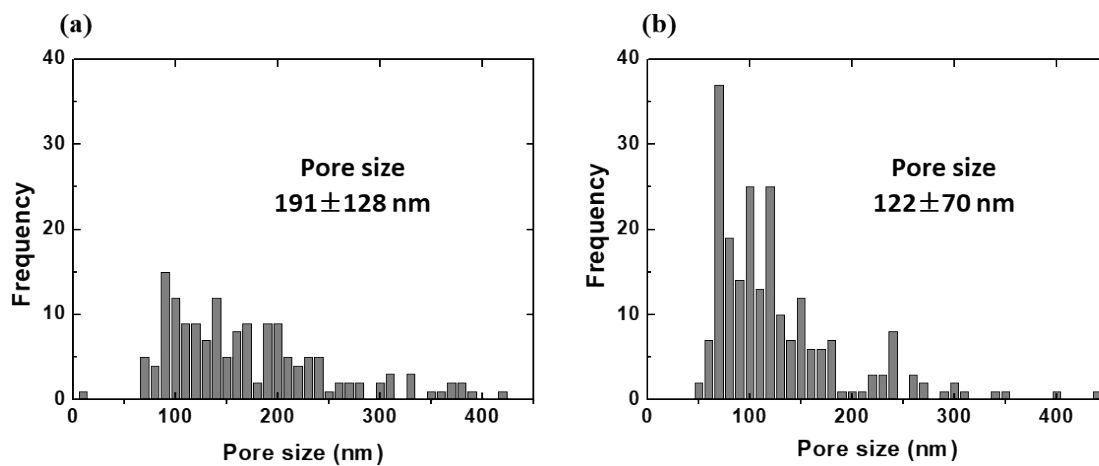


Figure S4. Size distribution histogram of pores on photo-polymerized bilayers of (a) DPPC/DiynPC (2:1) and (b) DPPC/DiynPC (4:1) mixtures.