

Lipid monolayer disruption caused by aggregated carbon nanoparticles

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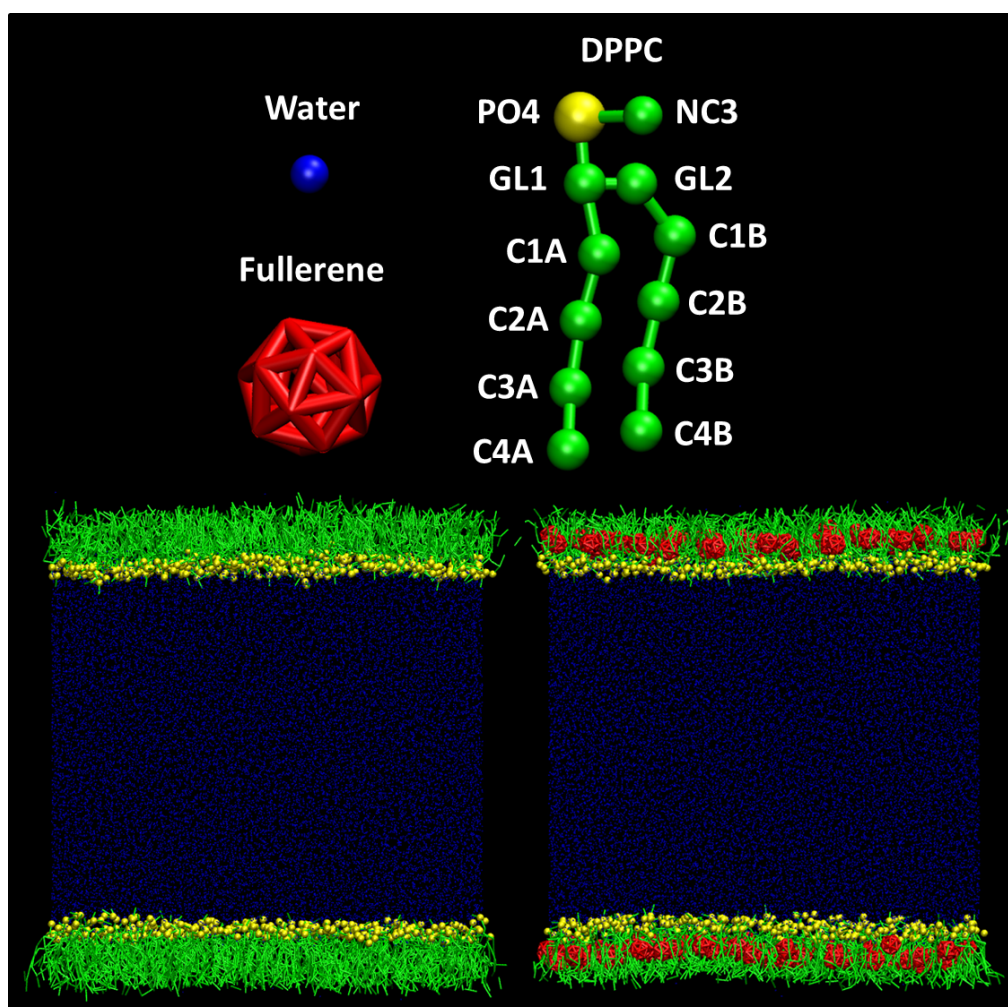


Figure S1. MARTINI molecular models for water, fullerene, and DPPC lipid molecules, and the system setup at the area per monolayer of 0.60 nm^2 with $[\text{C60}]/[\text{DPPC}]$ ratios of 0 (left) and 0.3 (right).

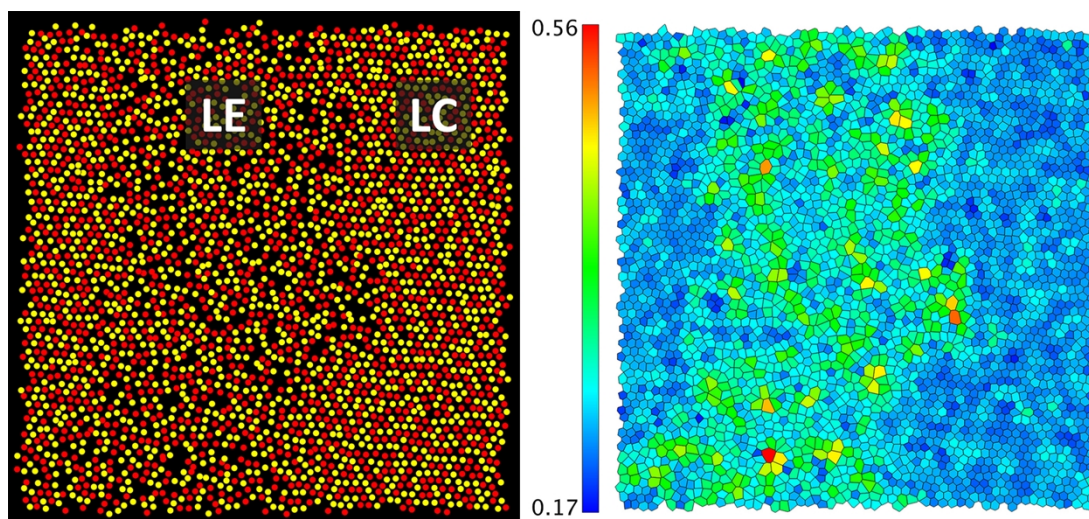


Figure S2. Left: Coexistence of LC and LE phases for a pure DPPC monolayer of 1600 molecules per leaflet at $0.52 \text{ nm}^2/\text{molecule}$. Red and yellow beads represent the C1A and C1B beads in DPPC molecules. Right: Voronoi tessellation using C1 beads in DPPC molecules. Colors indicate the size of Voronoi polygons in units of nm^2 .

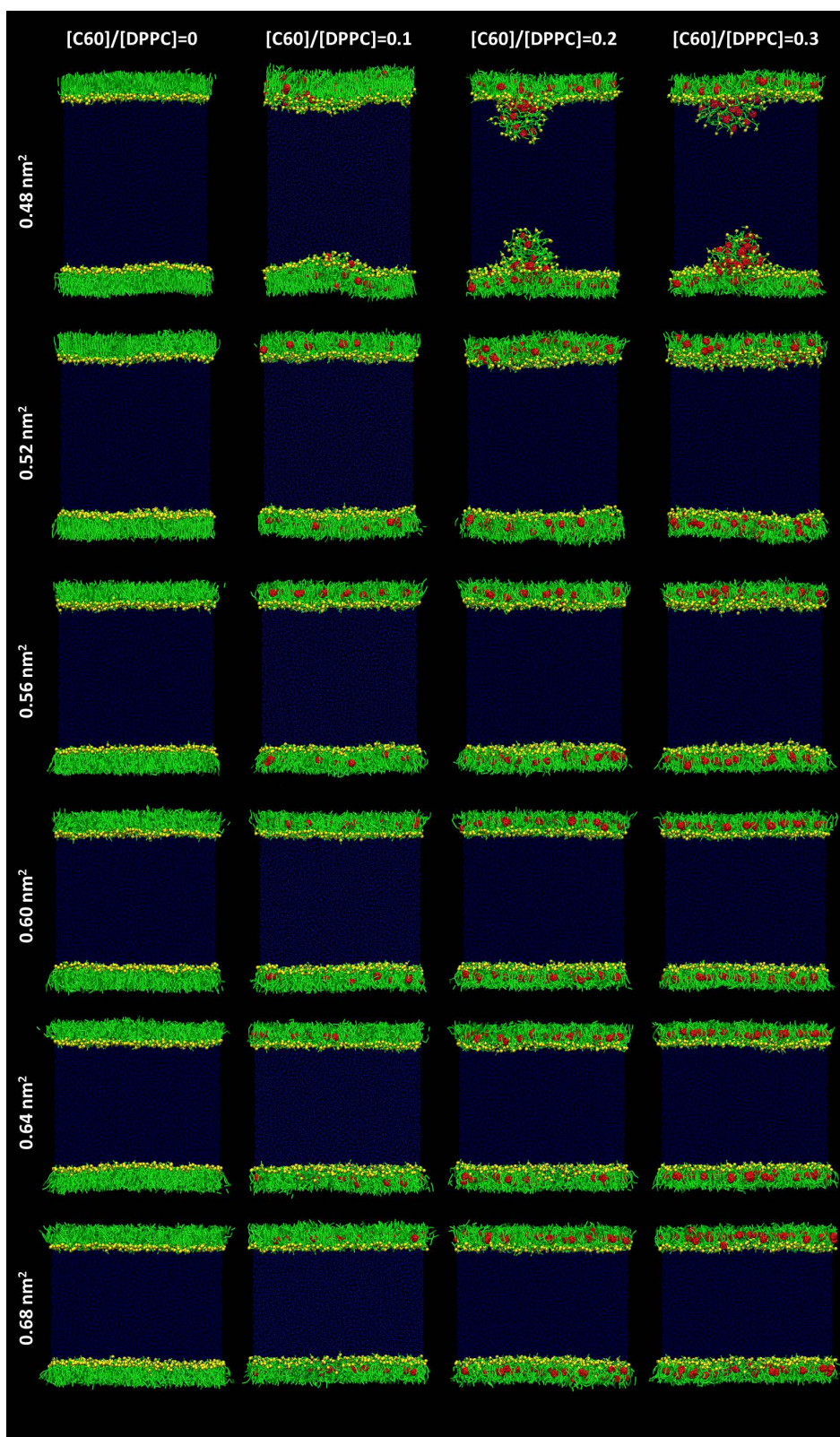


Figure S3. Snapshots illustrating the last frames of the systems in the xz -plane with 400 molecules/monolayer. Green: lipid tails, yellow: phosphate group in lipid heads, red: fullerene, and blue: water. Simulations were run for 5 μ s except four simulations with $[C60]/[DPPC]=0.2$ and 0.3 and at area per molecule of 0.48 and 0.52 nm² for 10 μ s.

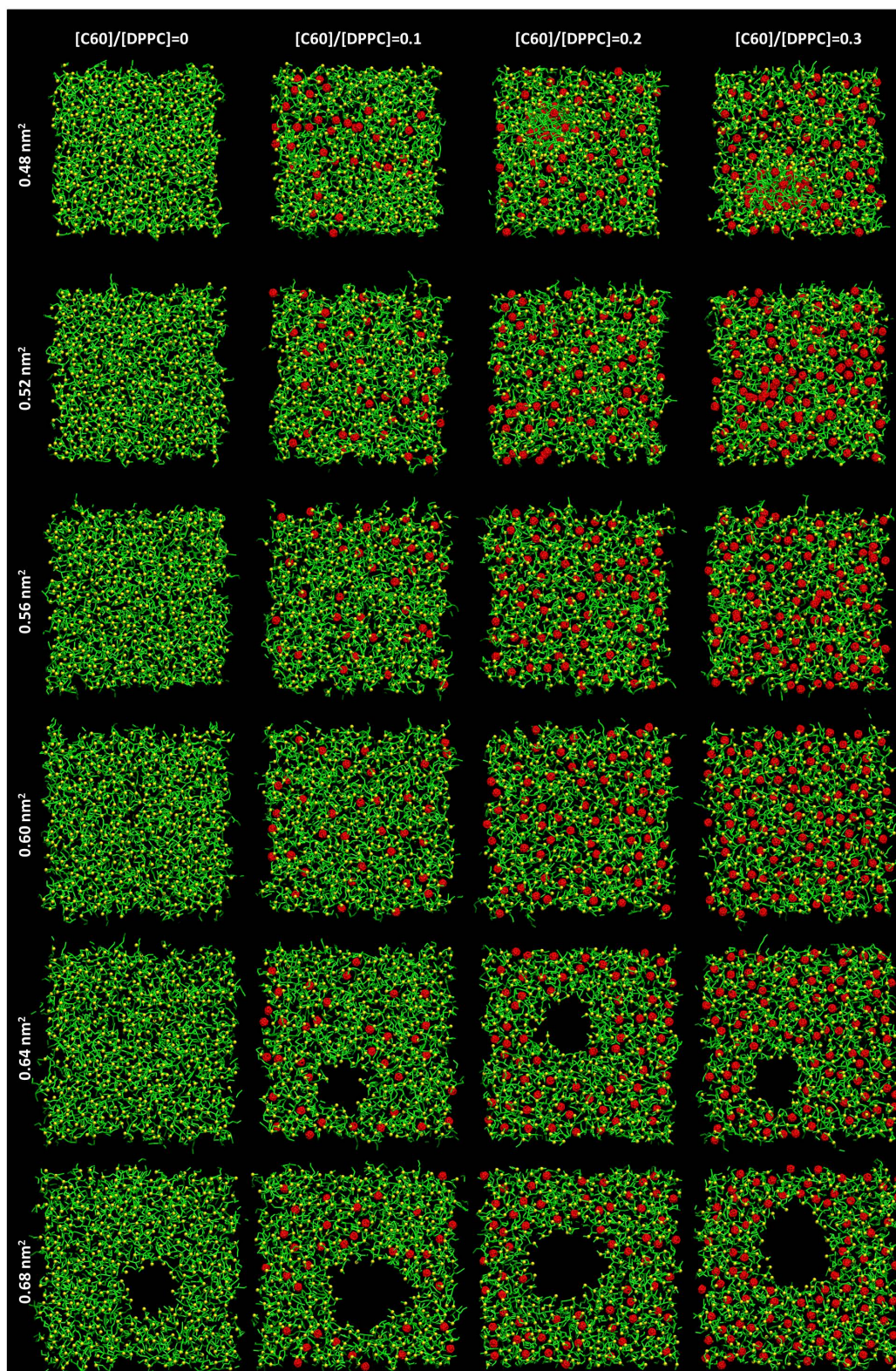


Figure S4. Snapshots illustrating the last frames of all systems in the xy -plane with 400 molecules/monolayer. Colors and simulation time are similar to Figure S3.

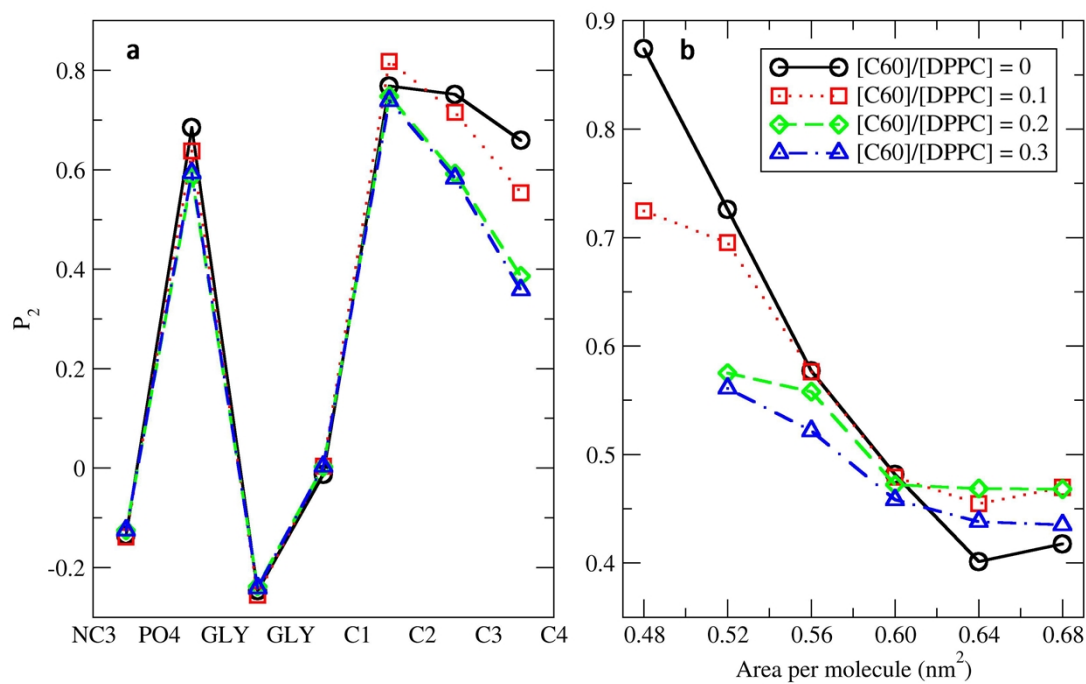


Figure S5. a) DPPC Bond order parameter profiles with respect to monolayer normal, calculated at the area per molecule of 0.52 nm². b) Average bond order parameter for the bonds C1-C2, C2-C3, and C3-C4 as a function of area per molecule at different concentrations of fullerene. The bond order parameter was not calculated when the monolayers collapsed (area per molecule of 0.48 nm² and [C60]/[DPPC] ratios 0.2 and 0.3). For atom numbering, see Figure S1.

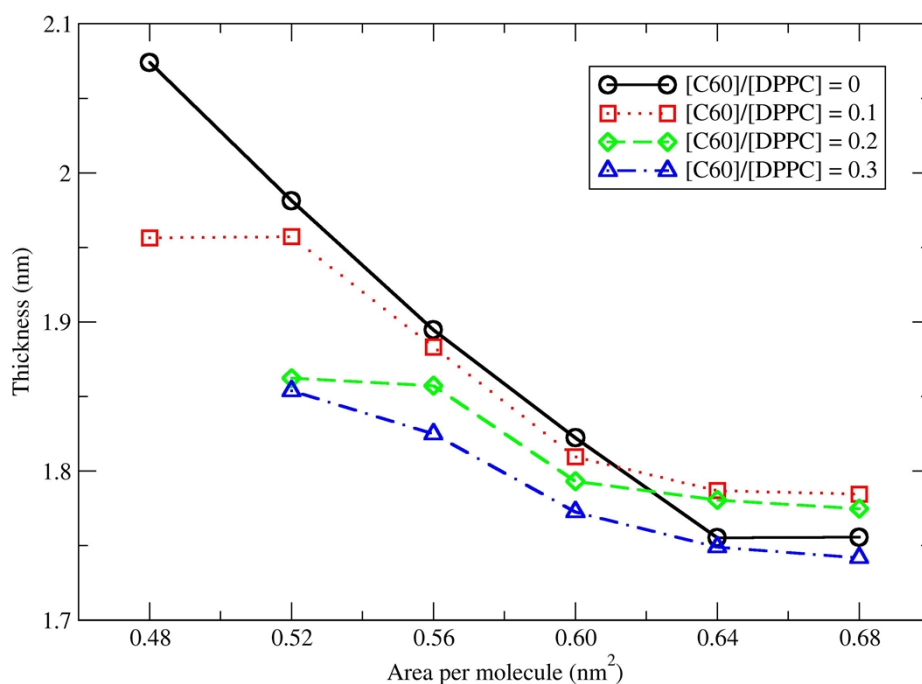


Figure S6. Monolayer thickness (defined by the distance between the center of mass (COM) of NC3 beads and the COM of C4A (for atom labels, see Fig. S1) beads) as a function of the area per molecule, with [C60]/[DPPC] ratios of 0, 0.1, 0.2 and 0.3. The thickness was not calculated when the monolayers collapsed (area per molecule of 0.48 nm² and [C60]/[DPPC] ratios 0.2 and 0.3).

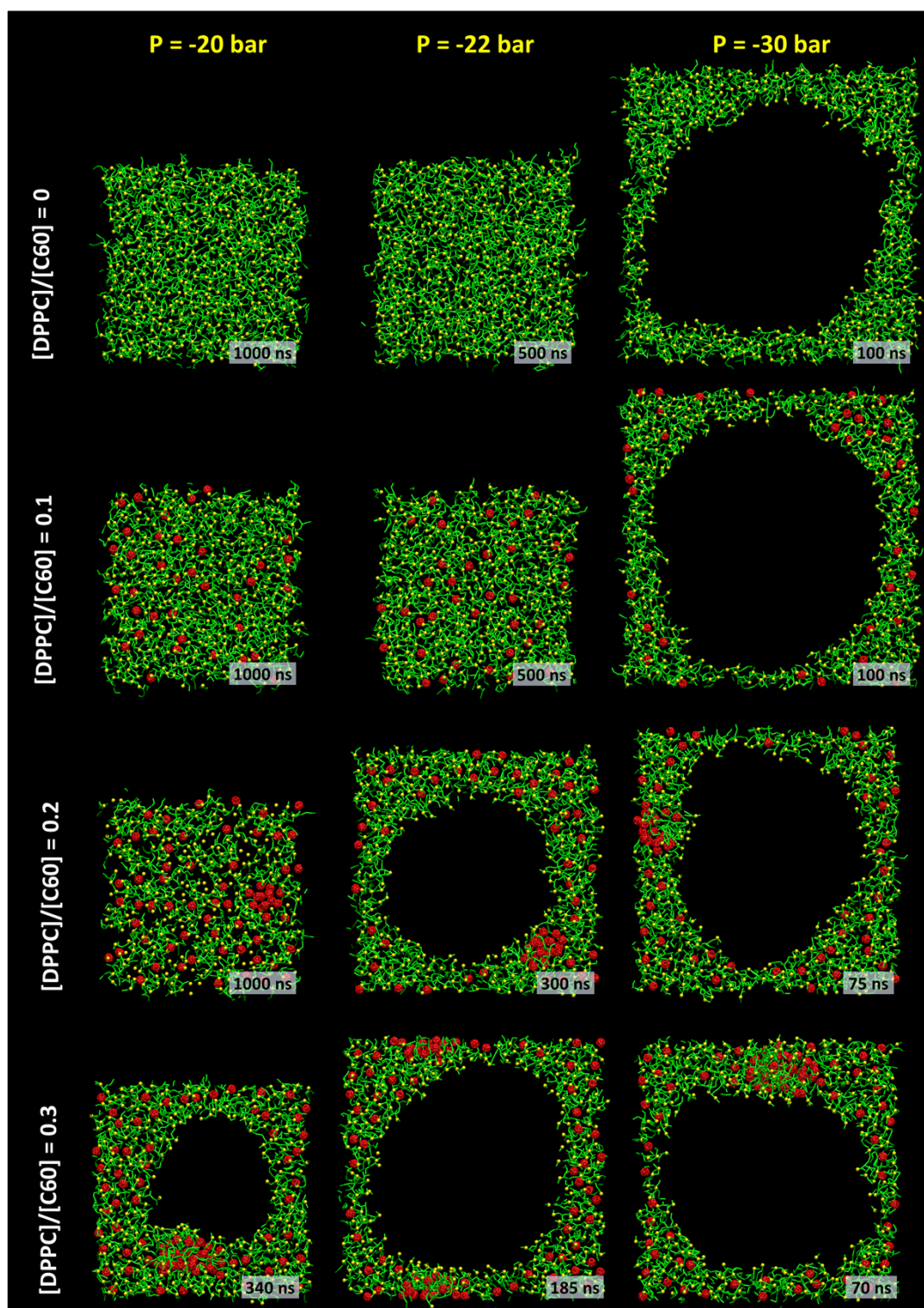


Figure S7. The pore formation in monolayer when the expansion with the semiisotropic lateral pressure at 20, 22, and 30 bar. Snapshots illustrated the systems of 400 molecules/monolayer in the xy -plane. Colors and simulation time are similar to Figure S3.

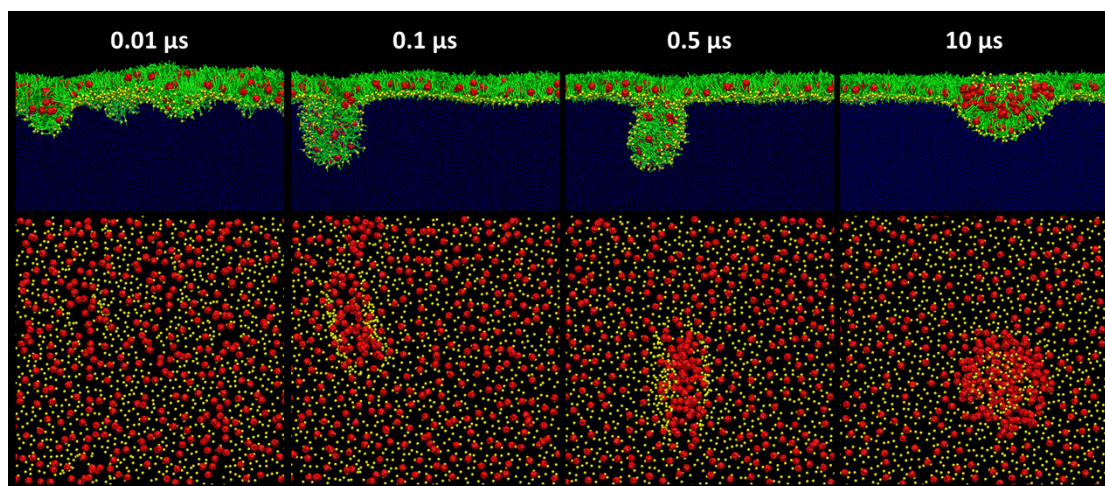


Figure S8. The time evolution of budding in monolayer. snapshots illustrated the systems of 1600 molecules/monolayer and $[\text{C60}]/[\text{DPPC}] = 0.3$. Colors are similar to Figure S3.