

# Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers

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## *Supporting information*

Sun-Joo Lee<sup>1</sup>, Paul H. Schlesinger<sup>2</sup>, Samuel A. Wickline<sup>3</sup>, Nathan A. Baker<sup>4</sup>

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<sup>1</sup> Department of Cell Biology and Physiology, Washington University in St. Louis

<sup>2</sup> Department of Cell Biology and Physiology, Washington University in St. Louis

<sup>3</sup> Department of Medicine, Washington University in St. Louis

<sup>4</sup> To whom correspondence should be addressed. Pacific Northwest National Laboratory, E-mail:  
[nathan.baker@pnnl.gov](mailto:nathan.baker@pnnl.gov)

## Molecular details of fusion initiation

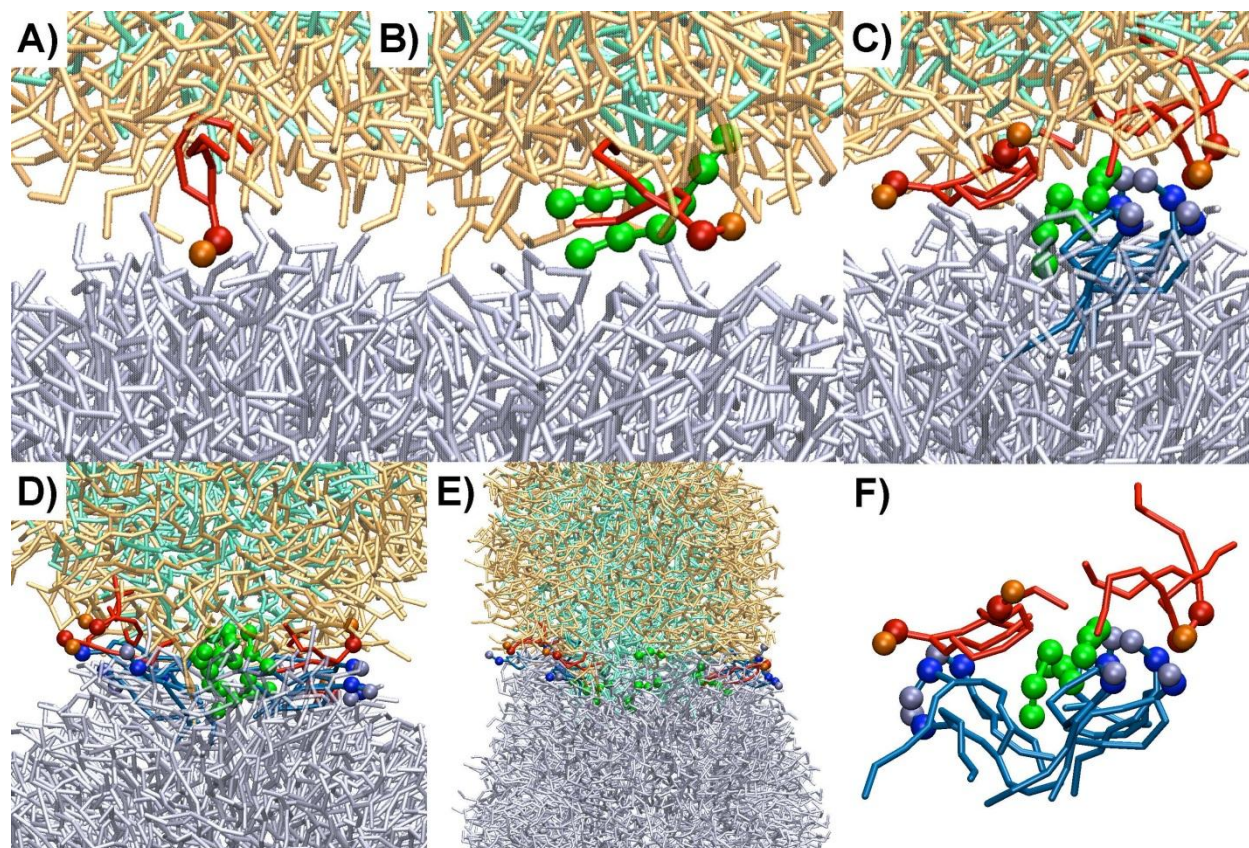


Figure S 1. Molecular details over the course of fusion. A) Initial monolayer perturbation that led to the fusion. B) Disruption of the monolayer via the protrusion of a lipid in alliance with PFOB molecules. C) Disruption of outer monolayer of the liposome and creation of hydrophobic pathway connecting the two particles. D) Flux of PFOB through the pathway to the hydrophobic lumen of the liposome and parallel stacking of lipid along the circumference at the initiation site. E) Widening of the pathway and massive flux of PFOB-NEP. F) The initial hydrophobic pathway as shown in C with other molecules omitted for clarity. Lipids and PFOBs that directly involved in the initial monolayer disruption are depicted in darker colors and thicker sticks and additional balls while the rest of the molecules are shown in thinner sticks and faint colors. PFOBs are shown in green and light green colors with the enclosing phospholipids in red and orange colors. The phospholipids of the liposomes are shown in blue and light blue.

## Fusion-induced changes in liposome geometry

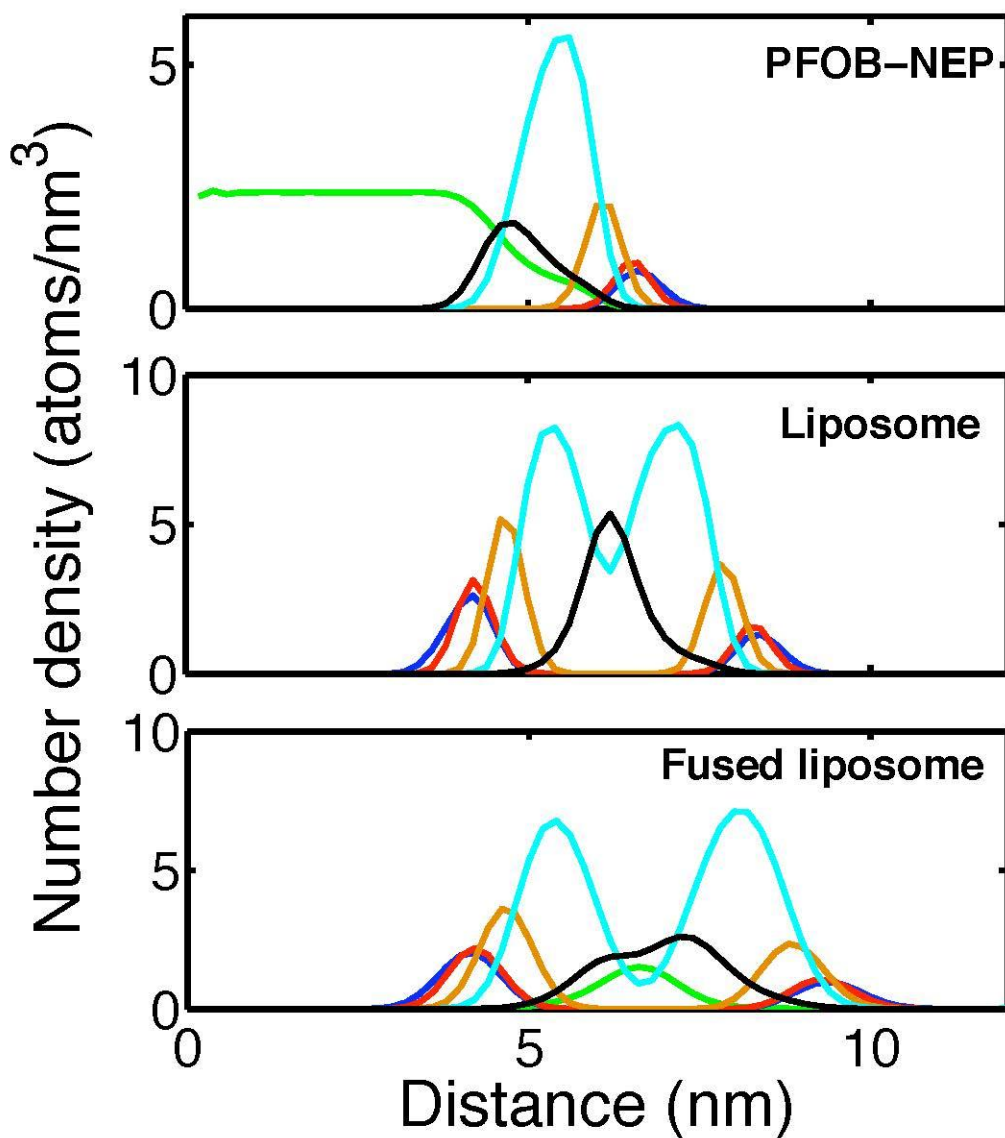


Figure S 2. Changes in liposome geometry after fusion. The top panel shows the number density of PFOB-NEP, the middle panel the number density of liposome, and the bottom panel the density of fused liposome. The density of PFOB is shown in green, choline group in blue, phosphate group in red, glycerol group in orange, lipid tails in cyan, terminal methyl group in black. The increase is observed in the bilayer thickness of the liposome after the fusion as a result of the absorption of PFOB into the intermonolayer space of the bilayer.