Supporting Information for Molecular Mechanism of Ionic Liquid Induced Membrane Disruption: Morphological Changes to Bilayers, Multi-Layers and Vesicles

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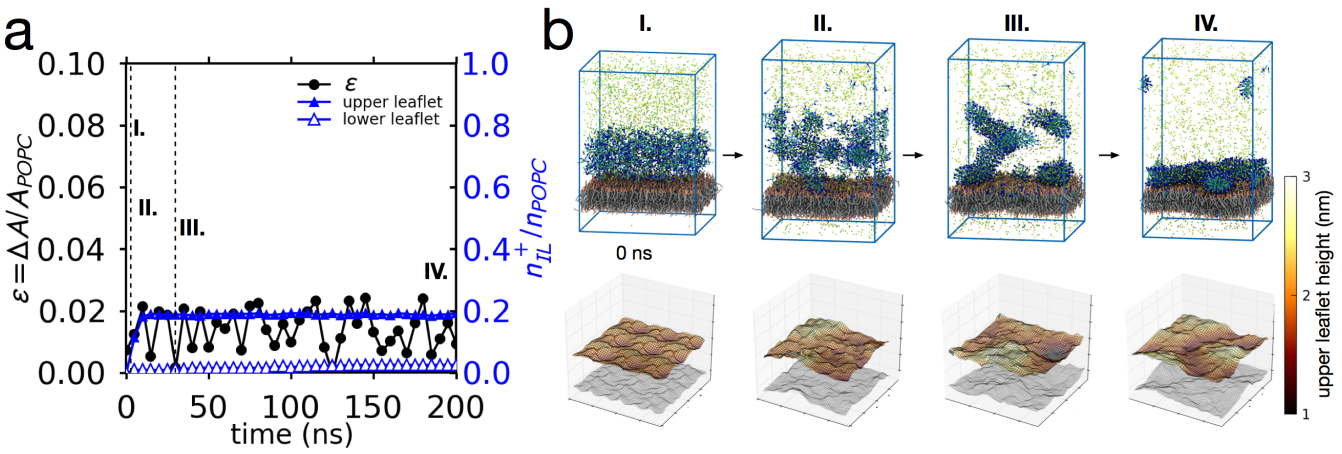

Figure S1 (a) Leaflet strain parameter and (b) snapshots from simulation of a POPC planar bilayer with [C_{10}mim]Cl. Cations rapidly form spherical micelles while a relatively small number of cations insert into the the top and bottom leaflet (II). The spherical micelles further fuse to form larger cylindrically shaped aggregates with a few of them coming into contact with the bilayer surface (III). After contact, IL cationic aggregates completely adsorb onto the bilayer surface. The leaflet strain parameter does not show signs of significant increase during course of the simulation. Cation insertion isotherms for (a) in the top and bottom leaflet are represented by the blue filled and open triangles respectively. Surface contour plots of the upper bilayer leaflet height (nm) corresponding to each simulation snapshot (I-IV) shown in (b) are plotted.

Table S1 Simulation conditions for each of the studied systems including: the system bilayer morphology, IL cation chain length (n), number of lipids (N_{POPC}), number of water beads (N_W), number of IL cations (N_{IL^+}), number of chloride ion beads (N_{Cl^-}), number of sodium ion beads (N_{Na^+}), final box dimension (in nm), and pressure coupling type.

system	n	N_{POPC}	N_W	(N_{IL^+})	N_{Cl^-}	N_{Na^+}	($L_x * L_y * L_z$)	pressure couple
planar	4	1152	87000	1000	1800	800	(20.9 * 20.9 * 21.9)	semi-isotropic
planar	10	1152	87000	1000	1800	800	(18.4 * 18.4 * 28.7)	semi-isotropic
double	4	2304	96000	2000	2800	800	(17.6 * 17.6 * 38.2)	semi-isotropic
vesicle	4	1512	151200	1600	2900	1300	(25.2 * 25.2 * 25.2)	isotropic
disk	10	1152	87000	1000	1800	800	(13.9 * 13.9 * 50.4)	semi-isotropic